10729542

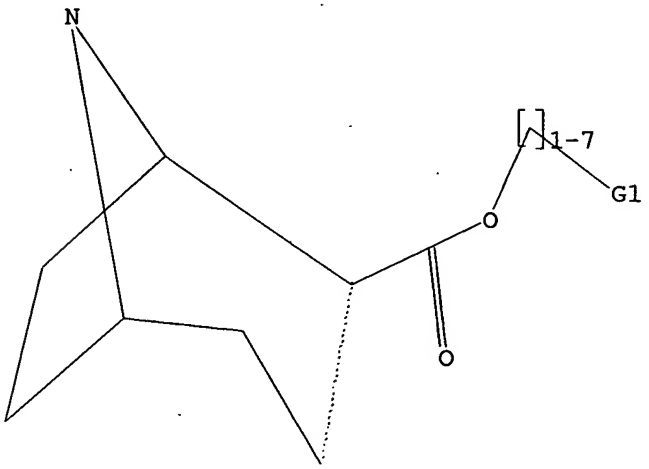
=> d his

(FILE 'HOME' ENTERED AT 12:02:07 ON 02 MAY 2005)

FILE 'REGISTRY' ENTERED AT 12:02:16 ON 02 MAY 2005
L1 STRUCTURE UPLOADED
L2 3 S L1
L3 135 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:03:36 ON 02 MAY 2005
L4 39 S L3
L5 28 S L4 NOT PHOSPH?

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S,N,X

Structure attributes must be viewed using STN Express query preparation.

=> d 1-28 bib abs hitstr

L5 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:93034 CAPLUS
DN 142:216950
TI Fluorescent Cocaine Probes: A Tool for the Selection and Engineering of Therapeutic Antibodies
AU Meijler, Michael M.; Kaufmann, Gunnar F.; Qi, Longwu; Mee, Jenny M.; Coyle, Avery R.; Moss, Jason A.; Wirsching, Peter; Matsushita, Masayuki; Janda, Kim D.
CS Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SO Journal of the American Chemical Society (2005), 127(8), 2477-2484
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal

LA English

AB Cocaine is a highly addictive drug, and despite intensive efforts, effective therapies for cocaine craving and addiction remain elusive. In recent years, we and others have reported advances in anti-cocaine immunopharmacotherapy based on specific antibodies capable of sequestering the drug before it reaches the brain. In an effort to obtain high affinity therapeutic anti-cocaine antibodies, either whole IgGs or other antibody constructs, fluorescence spectroscopic techniques could provide a means of assisting selection and engineering strategies. We report the synthesis of a series of cocaine-fluorophore conjugates (GNC-F1, GNC-F2, GNC-I) and the functional evaluation of these compds. against single-chain Fv antibodies obtained via crystallog. anal./engineering and against com. available anti-cocaine monoclonal antibodies with a wide range of cocaine-binding affinities. From these studies, we determined that the GNC-F2 fluorophore reproduced affinity consts. obtained using [3H]-labeled cocaine. We anticipate that the readily synthesized and nonradioactive GNC-F2 will find use both as a tool for bioimaging and in the high-throughput selection and engineering of potential therapeutic antibodies against cocaine.

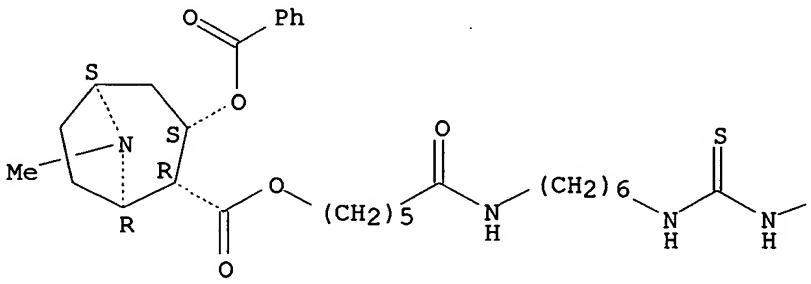
IT **843660-56-0P 843660-57-1P 843660-58-2P**
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fluorescent cocaine probes in selection and engineering of therapeutic antibodies)

RN 843660-56-0 CAPLUS

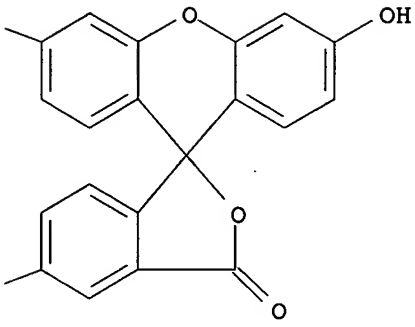
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 6-[[6-[[[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]thioxomethyl]amino]hexyl]amino]-6-oxohexyl ester, (1R,2R,3S,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



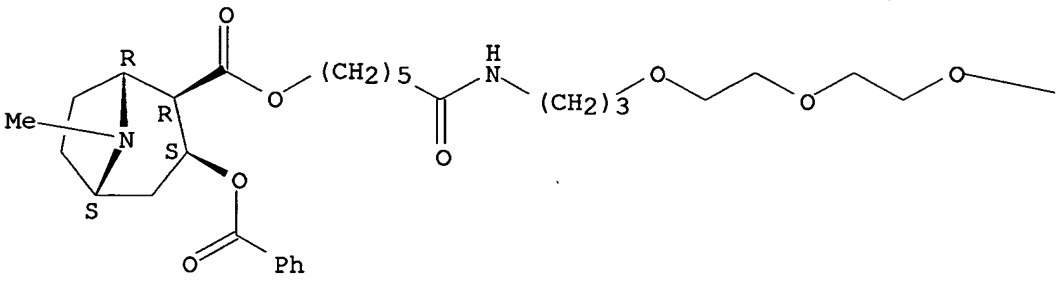
PAGE 1-B



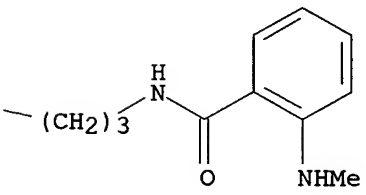
RN 843660-57-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 22-[2-(methylamino)phenyl]-6,22-dioxo-11,14,17-trioxa-7,21-diazadocos-1-yl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



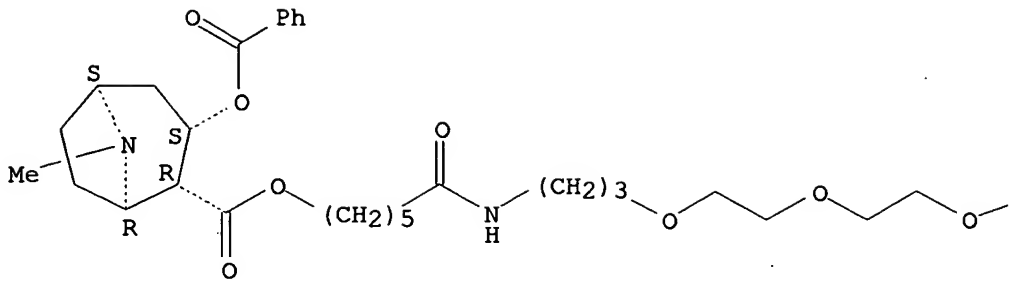
PAGE 1-B



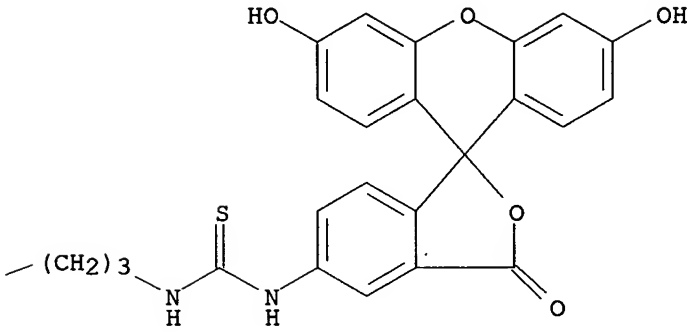
RN 843660-58-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 22-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)amino]-6-oxo-22-thioxo-11,14,17-trioxa-7,21-diazadocos-1-yl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

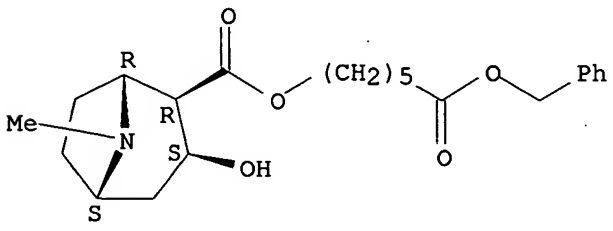


IT **173443-25-9P 173443-26-0P 173443-27-1P**
843660-60-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorescent cocaine probes in selection and engineering of therapeutic antibodies)

RN 173443-25-9 CAPLUS

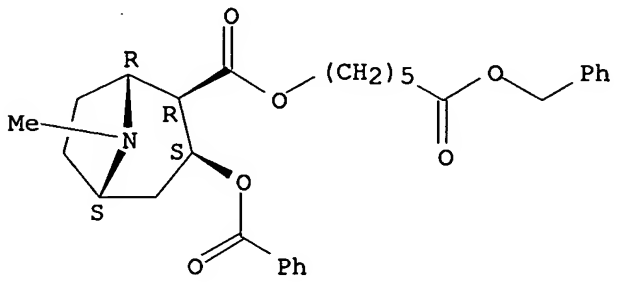
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 6-oxo-6-(phenylmethoxy)hexyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



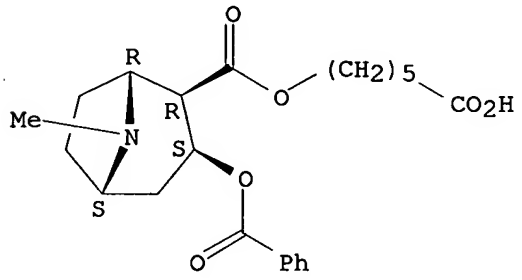
RN 173443-26-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 6-oxo-6-(phenylmethoxy)hexyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



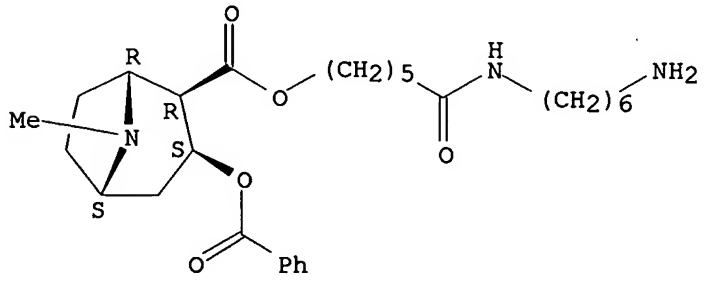
RN 173443-27-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 5-carboxypentyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 843660-60-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 6-[(6-aminohexyl)amino]-6-oxohexyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

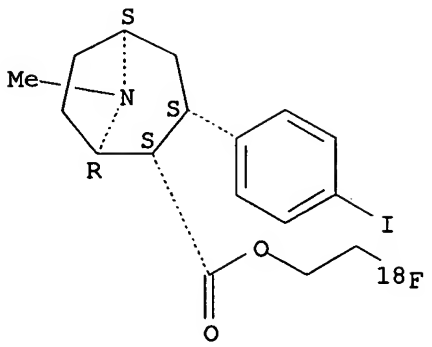
Absolute stereochemistry.



RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

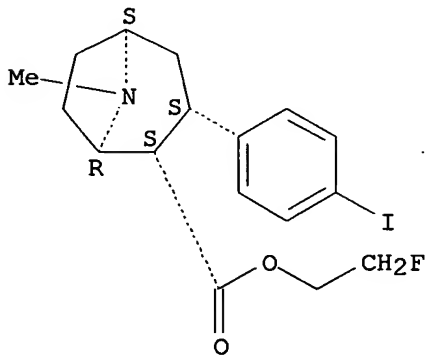
L5 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:1155647 CAPLUS
DN 142:341622
TI Synthesis and biodistribution of [18F]FE@CIT, a new potential tracer for the dopamine transporter
AU Mitterhauser, Markus; Wadsak, Wolfgang; Mien, Leonhard-Key; Hoepping, Alexander; Viernstein, Helmut; Dudczak, Robert; Kletter, Kurt
CS Department of Nuclear Medicine, Medical University of Vienna, Austria
SO Synapse (New York, NY, United States) (2004), Volume Date 2005, 55(2), 73-79
CODEN: SYNAET; ISSN: 0887-4476
PB Wiley-Liss, Inc.
DT Journal
LA English
AB In the last decade radiolabeled tropane analogs based on β-CIT have proven indispensable for the imaging of the dopamine transporter. However, further improvements in their pharmacodynamic and pharmacokinetic features are desirable. An important improvement, yielding in higher affinity to the dopamine transporter (DAT) vs. serotonin transporter (SERT), can be achieved by a simple replacement of the carboxylic Me ester group in β-CIT by a fluoroethyl ester. The preparation and ex vivo evaluation of this new β-CIT-analog ([18F]FE@CIT) is presented here. Precursor and standard were prepared from β-CIT and analyzed by spectroscopic methods. Yields of precursor and standard preparation were 61% and 42%, resp. [18F]FE@CIT was prepared by distillation of [18F]bromofluoroethane ([18F]BFE) and reaction with (1R-2-exo-3-exo)8-methyl-3-(4-iodo-phenyl)-8-azabicyclo[3.2.1] octane-2-carboxylic acid. After 10 min at 150°C the product was purified using a C-18 SepPak. The radiosynthesis evinced radiochem. yields of >90% (based on [18F]BFE), the specific radioactivity was >416 GBq/μmol. An average 30 μAh cyclotron irradiation yielded more than 2.5 GBq [18F]FE@CIT. For the ex vivo bioevaluation, 20 male Sprague-Dawley rats were sacrificed at 5, 15, 30, 60, and 120 min after injection. Organs were removed, weighed, and counted. For autoradiog. expts., transverse brain slices of about 100 μm were prepared The ex vivo evaluation showed highest brain uptake in striatal regions, followed by thalamus and cerebellum. The highest striatum to cerebellum ratio was 3.73 and the highest thalamus to cerebellum ratio was 1.65. Autoradiog. images showed a good and differentiated uptake in striatal regions with a good target-to-background ratio.
IT **848396-43-0P**
RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and biodistribution of [18F]fluoroethyl ester of β-CIT, a new potential tracer for the dopamine transporter)
RN 848396-43-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-(fluoro-18F)ethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **398497-81-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biodistribution of [18F]fluoroethyl ester of β-CIT, a new potential tracer for the dopamine transporter)
RN 398497-81-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

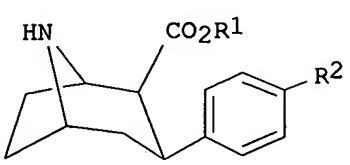
Absolute stereochemistry.



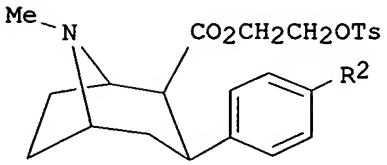
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:863118 CAPLUS
DN 142:38403
TI Synthesis and amine transporter affinities of novel phenyltropane derivatives as potential positron emission tomography (PET) imaging agents
AU Peng, Xuemei; Zhang, Ao; Kula, Nora S.; Baldessarini, Ross J.; Neumeyer, John L.
CS Medicinal Chemistry Laboratory, Alcohol and Drug Abuse Research Center, McLean Hospital, Harvard Medical School, Belmont, MA, 02478-9106, USA
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(22), 5635-5639
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.

DT Journal
LA English
GI



I



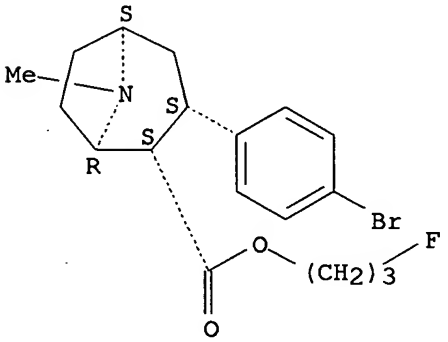
II

AB A series of novel fluoroalkyl-containing tropane derivs. were synthesized from cocaine. Novel compds. were evaluated for affinity and selectivity in competitive radioligand binding assays selective for cerebral serotonin (5-HT), dopamine (DA), and norepinephrine (NE) transporters (SERT, DAT, and NET). The nortropane-fluoroalkyl esters, I (R1 = (CH2)3F, R2 = Br; R1 = (CH2)2F, R2 = Br; R1 = (CH2)2F, R2 = I), were most potent for SERT (Ki: 0.18, 0.24, and 0.30 nM, resp.). Tosylate esters, II (R2 = Br, I), synthesized as precursors for [18F]-labeled, Positron Emission Tomog. (PET) imaging agents, also showed high affinity for DAT.

IT **805255-23-6P 805255-27-0P 805255-30-5P**
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and transporter bonding affinity of fluoroalkyl-containing tropane derivs.)

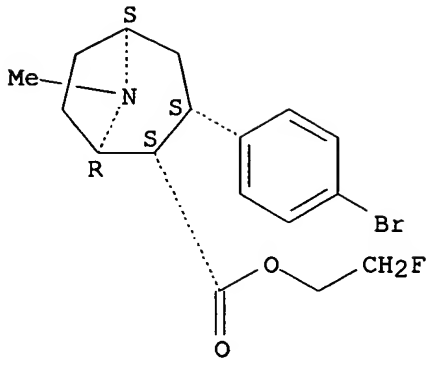
RN 805255-23-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-8-methyl-, 3-fluoropropyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



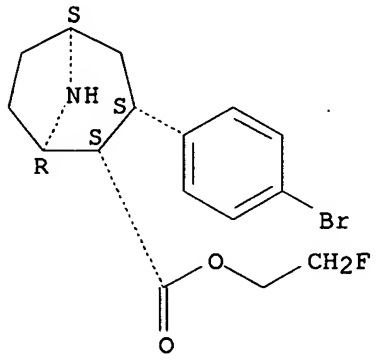
RN 805255-27-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-8-methyl-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



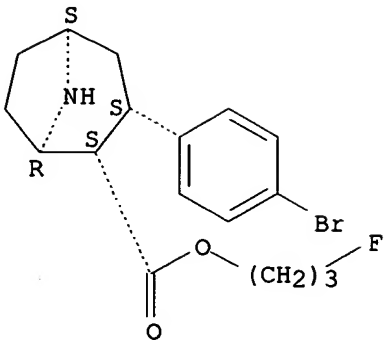
RN 805255-30-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



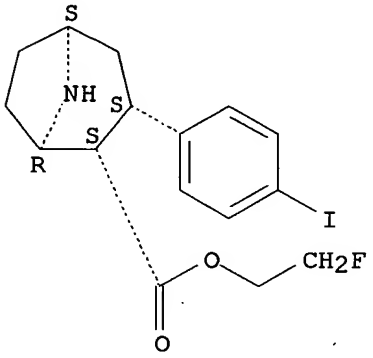
IT **805255-25-8P 805255-32-7P 805255-34-9P**
805255-44-1P 805255-46-3P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and transporter bonding affinity of fluoroalkyl-containing tropane derivs.)
RN 805255-25-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-, 3-fluoropropyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



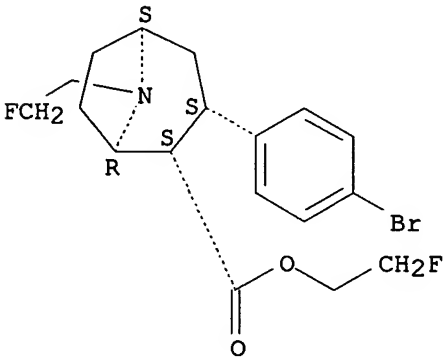
RN 805255-32-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



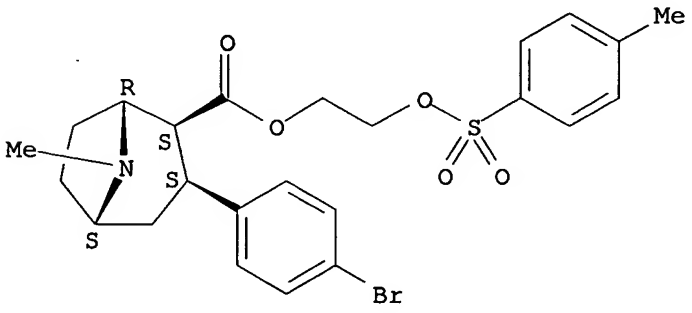
RN 805255-34-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-8-(2-fluoroethyl)-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



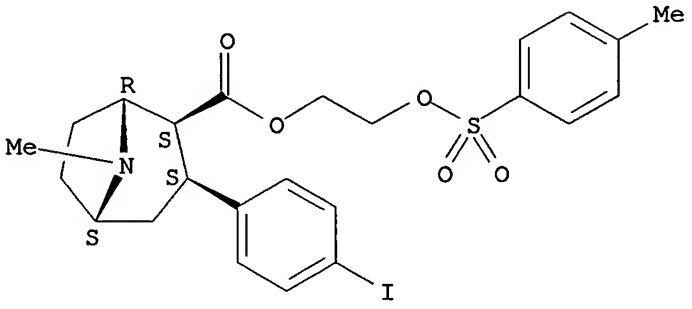
RN 805255-44-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-8-methyl-, 2-[[(4-methylphenyl)sulfonyl]oxy]ethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 805255-46-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-[[(4-methylphenyl)sulfonyl]oxy]ethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

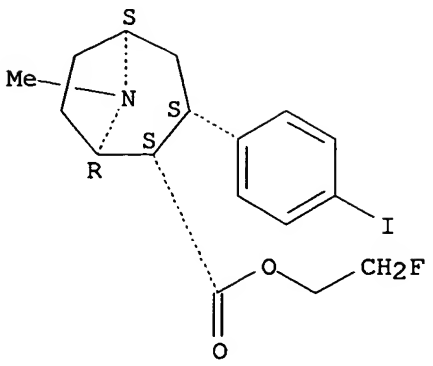
Absolute stereochemistry.



IT **398497-81-9P 805255-21-4P 805255-40-7P 805255-42-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and transporter bonding affinity of fluoroalkyl-containing tropane derivs.)

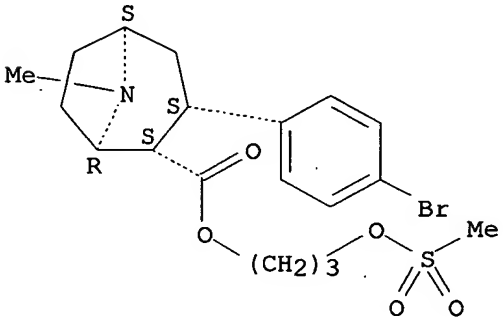
RN 398497-81-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



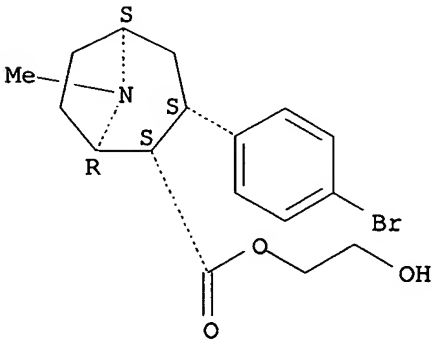
RN 805255-21-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-8-methyl-, 3-[(methylsulfonyl)oxy]propyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



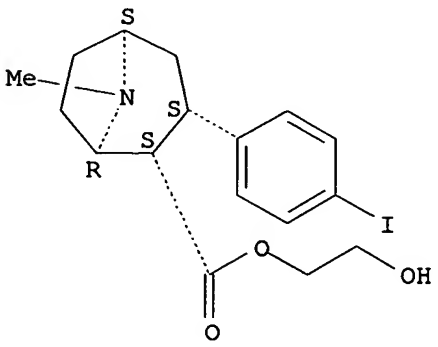
RN 805255-40-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-bromophenyl)-8-methyl-, 2-hydroxyethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 805255-42-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-hydroxyethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



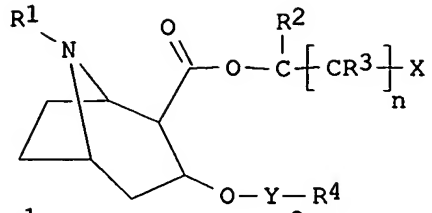
RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:515510 CAPLUS
DN 141:71754
TI Novel tropane esters and methods for producing and using them
IN Archer, Nicholas J.; Lewin, Anita H.
PA Entropin, Inc., USA
SO PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

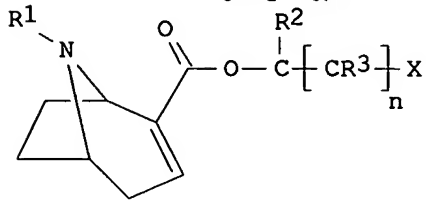
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004052888	A2	20040624	WO 2003-US38791	20031205
	WO 2004052888	A3	20040812		
	WO 2004052888	B1	20041021		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004171635	A1	20040902	US 2003-729542	20031205
PRAI	US 2002-431609P	P	20021205		

OS MARPAT 141:71754
GI

this appn



I



II

AB This invention relates to novel primary diol tropane esters and related compds., including methods for making and using those compds. The compds. of this invention are those of formula I or II (R1 = H, aryl, arylalkyl, alkyl, alkenyl, alkynyl, -CO-alkyl, -CO-aryl, and -CO-arylalkyl; R2, R3 independently = H, branched or unbranched alkyl, alkenyl, and alkynyl; R4 = H, branched or unbranched alkyl, alkenyl, and alkynyl, aryl, arylalkyl; X = OH, SH, amino, halogen; Y = CO or nothing; n = 0-6). Thus, cocaine hydrochloride in concentrated HCl was refluxed overnight, filtered and washed with di-Et ether to yield ecgonidine hydrochloride which was treated with an excess of 1,3-propanediol to give 1-hydroxy-3-Pr ecgonidine. These compds. may be used as therapeutic and prophylactic agents against diseases such as immunoregulatory disorders, neuromuscular disorders, joint disorders, connective tissue disorders, circulatory disorders and pain.

IT **709666-32-0P**

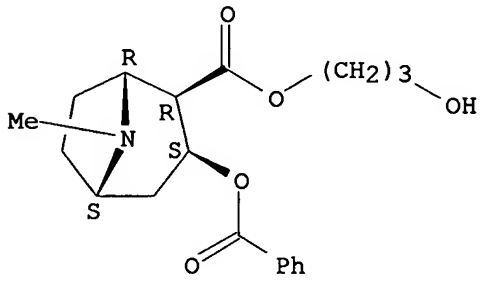
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of tropane esters as therapeutic agents for immunoregulatory disorders, neuromuscular disorders, joint disorders, connective tissue disorders, circulatory disorders and pain)

RN 709666-32-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 3-hydroxypropyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

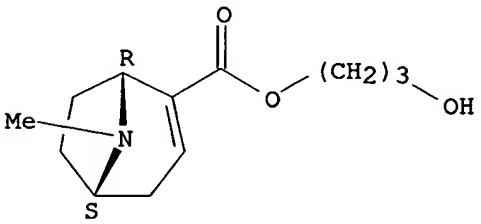
Absolute stereochemistry.



IT **709666-31-9P 709666-33-1P 709666-34-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tropane esters as therapeutic agents for immunoregulatory disorders, neuromuscular disorders, joint disorders, connective tissue disorders, circulatory disorders and pain)

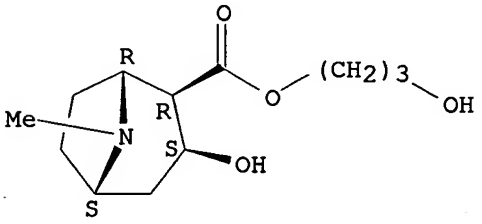
RN 709666-31-9 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 3-hydroxypropyl ester, (1R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 709666-33-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 3-hydroxypropyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

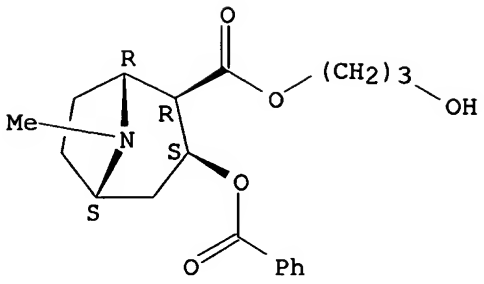


RN 709666-34-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 3-hydroxypropyl ester, (1R,2R,3S,5S)-, sulfate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

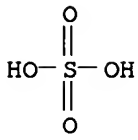
CRN 709666-32-0
CMF C19 H25 N O5

Absolute stereochemistry.



CM 2

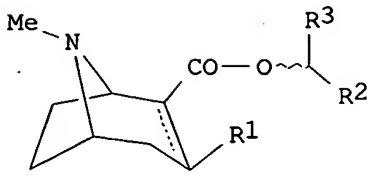
CRN 7664-93-9
CMF H2 O4 S



L5 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:182876 CAPLUS
DN 140:235927
TI Process for preparing hydroxyalkyl tropane esters
IN Lewin, Anita H.; Hayes, James P.; Zhong, Desong
PA Entropin, Inc., USA
SO PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004018464	A1	20040304	WO 2003-US26433	20030821
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004171834	A1	20040902	US 2003-646284	20030821
PRAI	US 2002-405433P	P	20020821		

OS CASREACT 140:235927
GI



I

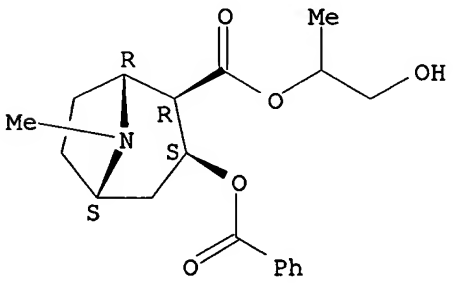
AB The present invention provides a method for preparing hydroxyalkyl tropane esters, such as I [dashed bond = single bond, double bond; R1 = H, OH, OCOPh; R2 = H, CH2OH; R3 = Me, CH(OH)Me], comprising: (a) contacting a tropane and 1,1'-carbonyldiimidazole to produce an activated tropane ester; (b) contacting the activated tropane ester with an excess of an alkanediol to form a reaction mixture; and (c) maintaining the reaction mixture at a temperature and for a sufficient time for the activated tropane ester to react with the alkanediol to form the corresponding hydroxyalkyl tropane ester. Thus, ecgonidine hydrochloride, obtained via refluxing cocaine hydrochloride with concentrated HCl, was reacted with 1,2-propanediol to afford 2-hydroxypropyl ecgonidine I [dashed bond = double bond, R1 = H, R2 = H, R3 = CH(OH)Me] and 1-hydroxy-2-Pr ecgonidine I [dashed bond = double bond, R1 = H, R2 = CH2OH, R3 = Me]. This method may be used to produce hydroxyalkyl derivs. of tropanes such as benzoylecgonine, ecgonine and ecgonidine.

IT **528840-36-0P**, 1-Hydroxy-2-propyl benzoylecgonine
528840-37-1P, 1-Hydroxy-2-propyl ecgonidine **611206-42-9P**, 2-Hydroxypropyl benzoylecgonine **611206-43-0P**, 2-Hydroxypropyl ecgonidine **666845-24-5P**, 2-Hydroxypropyl ecgonine **666845-26-7P**, 1-Hydroxy-2-propyl ecgonine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of hydroxyalkyl tropane esters)

RN 528840-36-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2-hydroxy-1-methylethyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

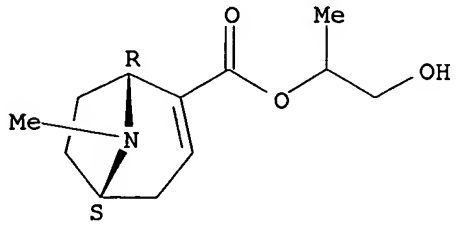
Absolute stereochemistry.



RN 528840-37-1 CAPLUS

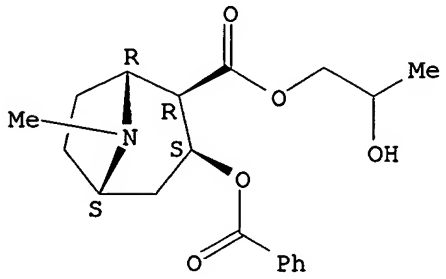
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 2-hydroxy-1-methylethyl ester, (1R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



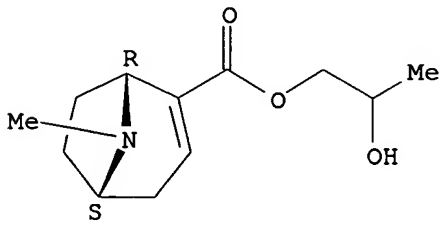
RN 611206-42-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2-hydroxypropyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



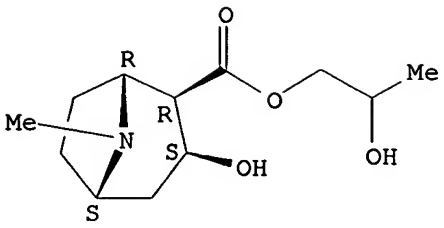
RN 611206-43-0 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 2-hydroxypropyl ester, (1R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



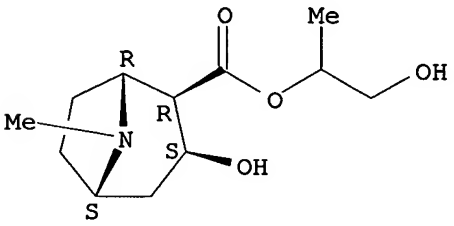
RN 666845-24-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 2-hydroxypropyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 666845-26-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 2-hydroxy-1-methylethyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

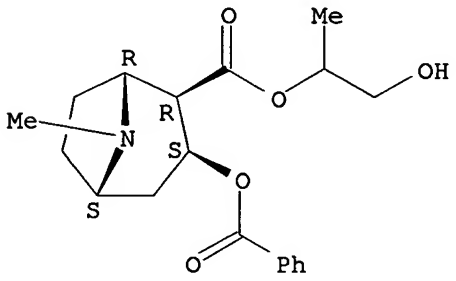
L5 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:904276 CAPLUS
DN 141:111320
TI Determination of the Dermal Penetration of Esterom Components Using Microdialysis Sampling
AU McDonald, Sarah; Lunte, Craig
CS Department of Chemistry, University of Kansas, Lawrence, KS, 66045, USA
SO Pharmaceutical Research (2003), 20(11), 1827-1834
CODEN: PHREEB; ISSN: 0724-8741
PB Kluwer Academic/Plenum Publishers
DT Journal
LA English
AB Esterom Solution, an investigational pharmaceutical product, is derived from the esterification of benzoylmethylecgonine (cocaine) in 1,2 propanediol. The resulting solution contains a mixture of components. Esterom Solution is intended to be a topical analgesic to relieve pain and increase the range of motion in patients suffering from acute inflammation of the shoulder or back. Although the components of Esterom are known, the components that are responsible for analgesia have only recently been identified. The purpose of this research is to evaluate which components have the ability to penetrate the skin, how much actually penetrates, and if and/or how each component is metabolized and distributed locally. Linear microdialysis probes were implanted into rat dermis. The individual components present in the Esterom Solution were applied sep. to the dermis directly over a probe. Dermal dialysis samples were collected to evaluate

the dermal penetration of each compound following topical application. Following a 10 mg/50 μL application, 1.8±0.6 mM benzoic acid was detected at the plateau after approx. 220 min. Following hydroxypropyl benzoic acid application, complete hydrolysis to benzoic acid was observed with a plateau concentration of 137±19 μM (150 min plateau). When applied sep., hydroxypropyl benzoylecgonine and ecgonine penetrate the skin with plateau concns. of 32±9 μM (15 h plateau) and 36±5 μM (150 min plateau) resp. Benzoylecgonine, the hydrolytic product of HP-BE, was also detected with a plateau concentration of 3.9±0.1 μM (16 h plateau) Applied topically, ecgonidine, methylecgonidine, benzoylecgonine, and hydroxypropyl ecgonidine were not detected. Of the components with analgesic activity, the only compound that penetrates the skin is hydroxypropyl benzoylecgonine. Dermal microdialysis was shown to be an effective technique to monitor the skin penetration of topically applied compds.

IT **528840-36-0 528840-37-1 611206-42-9**
611206-43-0
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(determination of dermal penetration of Esterom components using microdialysis
sampling)

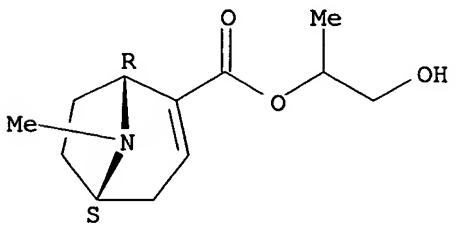
RN 528840-36-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2-hydroxy-1-methylethyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



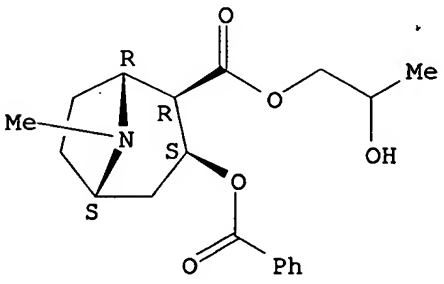
RN 528840-37-1 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 2-hydroxy-1-methylethyl ester, (1R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



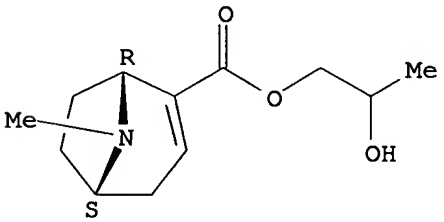
RN 611206-42-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2-hydroxypropyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 611206-43-0 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 2-hydroxypropyl ester, (1R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

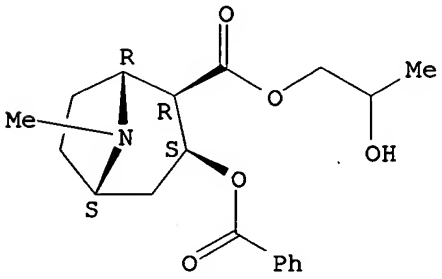
L5 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:503476 CAPLUS
DN 139:312548
TI Cyclodextrin-modified micellar electrokinetic chromatography for the analysis of esterom, a topical product consisting of hydrolyzed benzoylecgonine in propylene glycol
AU Razak, Jennifer L.; Doyen, Heidi J.; Lunte, Craig E.
CS Department of Chemistry, University of Kansas, Lawrence, KS, USA
SO Electrophoresis (2003), 24(11), 1764-1769
CODEN: ELCTDN; ISSN: 0173-0835
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB Esterom, a new drug currently in human clin. trials, is a mixture of compds. in a propylene glycol vehicle. It is being evaluated as a topical treatment to aid in the relief of muscle pain and to increase range of motion. Benzoylecgonine is the major component of esterom and there are

at least nine other minor constituents, including four hydroxypropyl esters that have multiple diastereomers. The aim of the study was to develop a capillary electrophoresis method for the simultaneous separation of the main components in Esterom, including the multiple proposed diastereomers of the esters. Due to the complex sample composition, the use of micelles and cyclodextrins as buffer modifiers was evaluated. A cyclodextrin-modified micellar electrokinetic chromatog. method was able to determine 7 of the 8 UV-active esterom components, with baseline separation of 7 of the 10 diastereomers of the hydroxypropyl esters.

IT **611206-42-9 611206-43-0**
RL: ANT (Analyte); ANST (Analytical study)
(determination of components of esterom by cyclodextrin-modified micellar electrokinetic chromatog.)

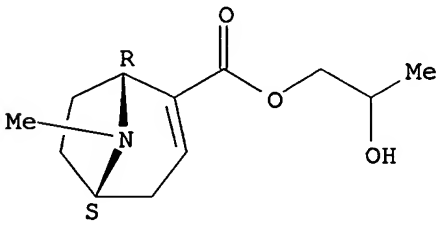
RN 611206-42-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2-hydroxypropyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 611206-43-0 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 2-hydroxypropyl ester, (1R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:492188 CAPLUS
DN 139:77878
TI Preparation of tropanes, their rhenium and technetium chelates and use as

radiopharmaceuticals and diagnostic agents

IN Turpin, Frederic; Mauclaire, Laurent; Masri, Fadi; Riche, Francoise; Du Moulinet D'Hardemare, Amaury

PA Schering Aktiengesellschaft, Germany

SO Fr. Demande, 65 pp.
CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2833952	A1	20030627	FR 2001-16867	20011226
FR 2833952	B1	20040326		
WO 2003055879	A2	20030710	WO 2002-IB5357	20021213
WO 2003055879	A3	20040617		

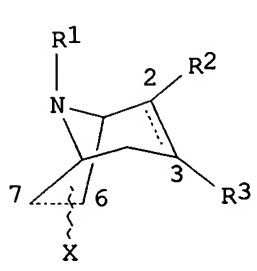
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI FR 2001-16867 A 20011226

OS MARPAT 139:77878

GI



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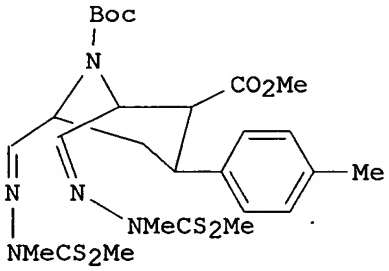
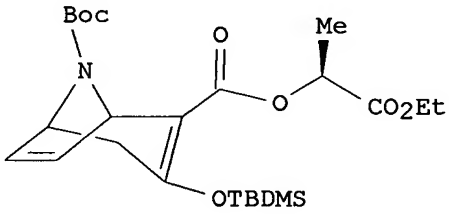


II



III

AB The present invention concerns tropanes (shown as I; variables defined below; e.g. II), their metal chelates with rhenium and technetium (e.g. Tc oxo and nitrido complexes with II), methods of preparation of the tropanes and their chelates, and uses as radiopharmaceuticals and diagnostic agents,

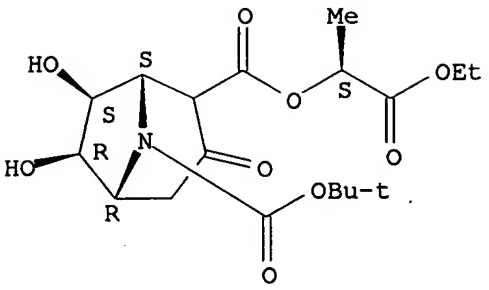
e.g. visualization of reuptake of dopamine or serotonin. For I: X = a compound of chelation of a metal or a metal complex, carbons 6 and 7 being bonded or not; R1 is an alkyl or a alkenyl; R2 is COOZ (Z = H, alkyl); R3 = Ph, phenylalkyl or phenylalkenyl, benzoate or oxo; the connection between carbons 2 and 3 is a simple or double bond. The portions of X bonded to carbons 6 and 7 may be, for example, :NN(R7)CS2Me (R7 = H, Me). For example, II was prepared in a multistep synthesis starting from N-Bocpyrrole and (1S)-2-ethoxy-1-methyl-2-oxoethyl 3-(tert-butyldimethylsiloxy)-2-diazo-3-oxo-3-butenoate (prepns. described) involving the following intermediates: (1S)-2-ethoxy-1-methyl-2-oxoethyl (1R,5R)-8-[(1,1-dimethylethoxy)carbonyl]-3-(tert-butyldimethylsiloxy)-8-azabicyclo[3.2.1]octa-2,6-diene-2-carboxylate (shown as III, 75%), (1S)-2-ethoxy-1-methyl-2-oxoethyl (1R,5R)-8-[(1,1-dimethylethoxy)carbonyl]-8-azabicyclo[3.2.1]oct-6-en-3-one-2-carboxylate, (1S)-2-ethoxy-1-methyl-2-oxoethyl (1R,5R)-8-[(1,1-dimethylethoxy)carbonyl]-3-(trifluoromethanesulfonyloxy)-8-azabicyclo[3.2.1]octa-2,6-diene-2-carboxylate (22%), (1S)-2-ethoxy-1-methyl-2-oxoethyl (1R,5R)-8-[(1,1-dimethylethoxy)carbonyl]-3-(p-tolyl)-8-azabicyclo[3.2.1]octa-2,6-diene-2-carboxylate (33%), Me (1R,5R)-8-[(1,1-dimethylethoxy)carbonyl]-3-(p-tolyl)-8-azabicyclo[3.2.1]octa-2,6-diene-2-carboxylate (95%), Me (1R,2R,3R,5R)-8-[(1,1-dimethylethoxy)carbonyl]-3-(p-tolyl)-8-azabicyclo[3.2.1]oct-6-ene-2-carboxylate (85%), Me (1R,2R,3R,5R,6R,7R)-8-[(1,1-dimethylethoxy)carbonyl]-6,7-dihydroxy-3-(p-tolyl)-8-azabicyclo[3.2.1]octane-2-carboxylate (99%), and Me (1R,2R,3R,5R)-6-[(1,1-dimethylethoxy)carbonyl]-1,5-diformyl-3-(p-tolyl)-6-azacyclohexane-2-carboxylate (70%). Pharmacol. testing of Tc complexes of tropane derivs. yielded the following results: preinjection of GBR 12909 (specific inhibitor of dopamine transport) in rats prevented their fixation in the striatum; in vitro competitive studies on cerebral membranes with radiolabeled GBR 12925, paroxetine and nisoxetine showed the Tc complexes to have good affinity and specificity for dopamine transport; in vivo kinetic studies of cerebral distribution in a primate shows the complexes to be useful for visualization of dopamine transport; they pass the hemato-encephalic barrier and accumulate preferentially in the striatum with an elevated striatum/cerebellum ratio.

IT **549506-08-3P 549506-09-4P 549506-10-7P**
549506-13-0P 549506-14-1P 549506-15-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tropanes, their rhenium and technetium chelates and use as radiopharmaceuticals and diagnostic agents)

RN 549506-08-3 CAPLUS

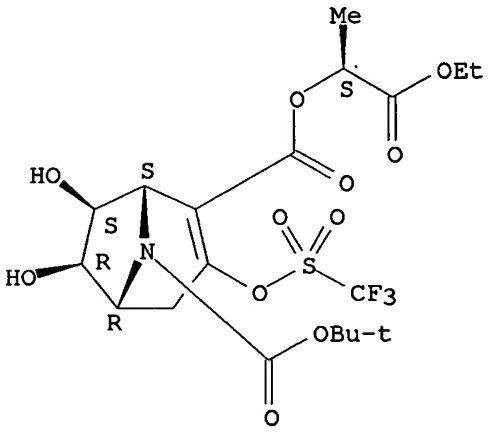
CN 8-Azabicyclo[3.2.1]octane-2,8-dicarboxylic acid, 6,7-dihydroxy-3-oxo-, 8-(1,1-dimethylethyl) 2-[(1S)-2-ethoxy-1-methyl-2-oxoethyl] ester, (1S,5R,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



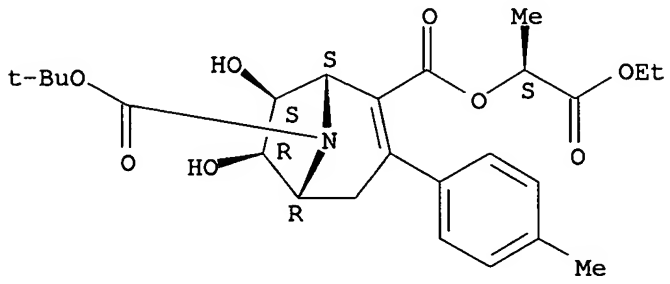
RN 549506-09-4 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2,8-dicarboxylic acid, 6,7-dihydroxy-3-[[(trifluoromethyl)sulfonyl]oxy]-, 8-(1,1-dimethylethyl) 2-[(1S)-2-ethoxy-1-methyl-2-oxoethyl] ester, (1S,5R,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



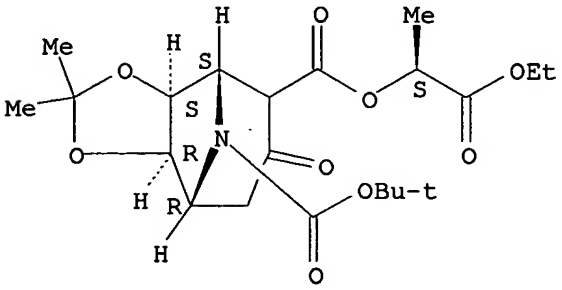
RN 549506-10-7 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2,8-dicarboxylic acid, 6,7-dihydroxy-3-(4-methylphenyl)-, 8-(1,1-dimethylethyl) 2-[(1S)-2-ethoxy-1-methyl-2-oxoethyl] ester, (1S,5R,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



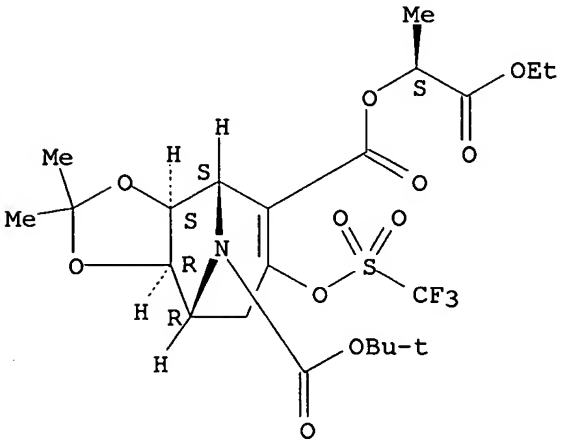
RN 549506-13-0 CAPLUS
CN 4H-Cyclohepta-1,3-dioxol-4,8-imine-5,9-dicarboxylic acid, hexahydro-2,2-dimethyl-6-oxo-, 9-(1,1-dimethylethyl) 5-[(1S)-2-ethoxy-1-methyl-2-oxoethyl] ester, (3aS,4S,8R,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



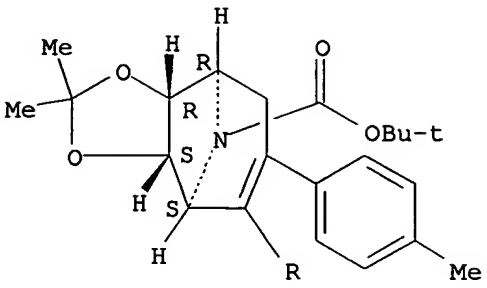
RN 549506-14-1 CAPLUS
CN 4H-Cyclohepta-1,3-dioxol-4,8-imine-5,9-dicarboxylic acid, 3a,7,8,8a-tetrahydro-2,2-dimethyl-6-[[(trifluoromethyl)sulfonyl]oxy]-, 9-(1,1-dimethylethyl) 5-[(1S)-2-ethoxy-1-methyl-2-oxoethyl] ester, (3aS,4S,8R,8aR)- (9CI) (CA INDEX NAME)

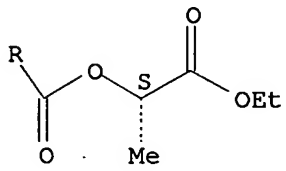
Absolute stereochemistry.



RN 549506-15-2 CAPLUS
CN 4H-Cyclohepta-1,3-dioxol-4,8-imine-5,9-dicarboxylic acid, 3a,7,8,8a-tetrahydro-2,2-dimethyl-6-(4-methylphenyl)-, 9-(1,1-dimethylethyl) 5-[(1S)-2-ethoxy-1-methyl-2-oxoethyl] ester, (3aS,4S,8R,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:396882 CAPLUS
DN 138:401953
TI Novel benzoylecgonine compositions and methods for producing them
IN Archer, Nicholas James
PA Entropin, Inc., USA
SO PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003042209	A1	20030522	WO 2002-US36384	20021113
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003144317	A1	20030731	US 2002-294858	20021113
	US 6790857	B2	20040914		
	EP 1444230	A1	20040811	EP 2002-789620	20021113
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	JP 2005509035	T2	20050407	JP 2003-544045	
PRAI	US 2001-348882P	P	20011113		
	WO 2002-US36384	W	20021113		

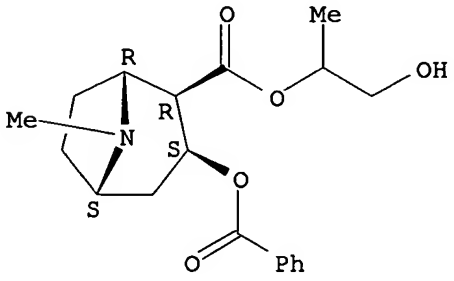
AB This invention provides a method for preparing a benzoylecgo

comprising the steps of: (a) contacting benzoylmethylecgonine and propylene glycol in the presence or absence of water to form a reaction mixture; (b) maintaining the reaction mixture at a temperature between about 50° and 100° C; and (c) subsequently or simultaneously removing water from the reaction mixture This invention also provides novel benzoylecgonine and methods for producing them.

IT **528840-36-0P 528840-37-1P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of benzoylecgonine derivs. from cocaine and propylene glycol)

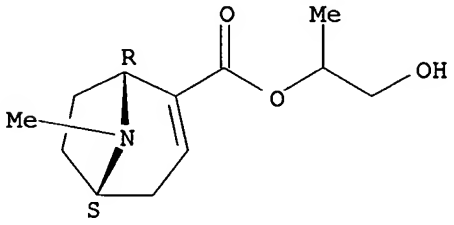
RN 528840-36-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2-hydroxy-1-methylethyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 528840-37-1 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 2-hydroxy-1-methylethyl ester, (1R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

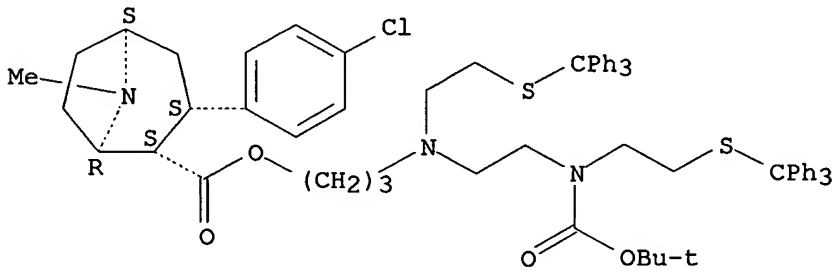


RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:162625 CAPLUS
DN 139:77836
TI S-Trityl protection of bis-amino bis-thiol (BAT) chelator enables flexible derivatisation and facile labelling with technetium-99m
AU Cleynhens, Bernard J.; Bormans, Guy M.; Vanbilloen, Hubert P.; Vanderghinste, Dominique V.; Kieffer, Davy M.; de Groot, Tjibbe J.;

Verbruggen, Alfons M.
CS Laboratory for Radiopharmaceutical Chemistry and Nuclear Medicine, University of Leuven, Louvain, B-3000, Belg.
SO Tetrahedron Letters (2003), 44(12), 2597-2600
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 139:77836
AB The authors have coupled S,S'-bis-trityl N-BOC protected 1,2-ethylenedicysteamine, a bis-amino bis-thiol (BAT) tetraligand, via a propylene or ethylene spacer to several biol. active mols. including 2-nitroimidazole, desethylflumazenil, a beta-CIT analog, glucose and 2-(2'-hydroxy-4'-aminophenyl)-1,3-benzothiazole. The conjugates were efficiently labeled with 99mTc by consecutive heating of the S,S'-bis-trityl protected ligand in HCl followed by neutralisation and heating in the presence of 99mTc-tartrate. The S,S'-bis-trityl BAT chelator is an interesting synthon that allows both flexible derivatisation with various biol. active mols. and facile labeling with Tc-99m.
IT **549514-77-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 549514-77-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, 3-[[2-[[(1,1-dimethylethoxy)carbonyl][2-[(triphenylmethyl)thio]ethyl]amino]ethyl][2-[(triphenylmethyl)thio]ethyl]amino]propyl ester, (1R,2S,3S,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

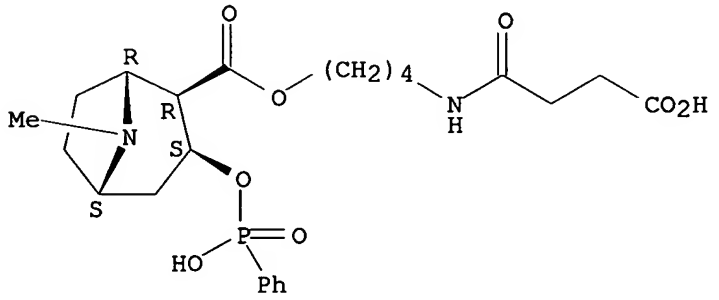


RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:787415 CAPLUS
DN 138:319388
TI Anticocaine catalytic antibodies
AU Deng, Shi Xian; de Prada, Paloma; Landry, Donald W.
CS Department of Medicine, Division of Clinical Pharmacology and Experimental Therapeutics, Columbia University, New York, NY, 10032, USA
SO Journal of Immunological Methods (2002), 269(1-2), 299-310
CODEN: JIMMBG; ISSN: 0022-1759
PB Elsevier Science B.V.

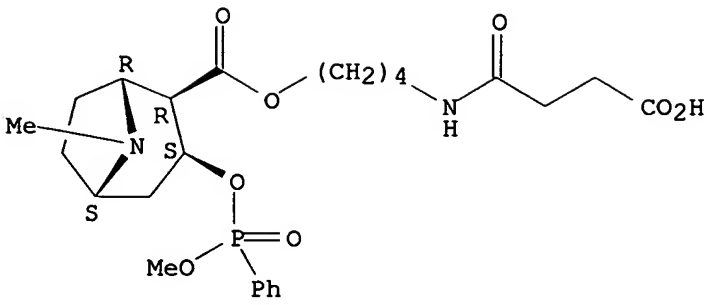
DT Journal
LA English
AB Cocaine mediates its reinforcing and toxic actions through a "loss of function" effect at multiple receptors. The difficulties inherent in blocking a pleiotropic blocker pose a great obstacle for the classical receptor-antagonist approach and have contributed to the failure (to date) to devise specific treatments for cocaine overdose and addiction. As an alternative, we have embarked on an investigation of catalytic antibodies, a programmable class of artificial enzyme, as "peripheral blockers"-agents designed to bind and degrade cocaine in the circulation before it partitions into the central nervous system to exert reinforcing or toxic effects. We synthesized transition-state analogs of cocaine's hydrolysis at its benzoyl ester, immunized mice, prepared hybridomas and developed the first anticocaine catalytic antibodies with the capacity to degrade cocaine to nonreinforcing, nontoxic products. We subsequently identified several families of anticocaine catalytic antibodies and found that the most potent antibody possessed sufficient activity to block cocaine-induced reinforcement, organ dysfunction and sudden death in rodent models of addiction, toxicity and overdose, resp. With the potential to promote cessation of use, prolong abstinence and provide a treatment for acute overdose, the artificial enzyme approach comprehensively responds to the problem of cocaine.
IT **324015-66-9P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(anticocaine catalytic antibodies alter cocaine hydrolysis and toxicity)
RN 324015-66-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(hydroxyphenylphosphinyl)oxy]-8-methyl-, 4-[(3-carboxy-1-oxopropyl)amino]butyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



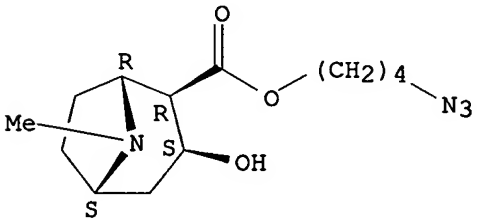
IT **152241-57-1P 152241-60-6P 152241-61-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of cocaine transition state analogs)
RN 152241-57-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(methoxyphenylphosphinyl)oxy]-8-methyl-, 4-[(3-carboxy-1-oxopropyl)amino]butyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



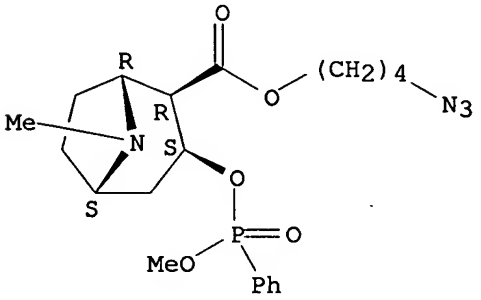
RN 152241-60-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 4-azidobutyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 152241-61-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(methoxyphenylphosphinyl)oxy]-8-methyl-, 4-azidobutyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:872207 CAPLUS
DN 136:167538

10729542

TI Synthesis and binding affinities of 2β-(3-iodoallyloxycarbonyl)-3β-(4-substituted-aryl)tropane analogues as ligands for the dopamine transporter studies

AU Chung, Kyoo-Hyun; Lim, Choong Hwan; Lee, Dong Reyoul; Jin, Changbae; Chi, Dae Yoon

CS Department of Chemistry, Inha University, Namgu, Inchon, 402-751, S. Korea

SO Bioorganic & Medicinal Chemistry Letters (2001), 11(23), 3077-3080
CODEN: BMCLE8; ISSN: 0960-894X

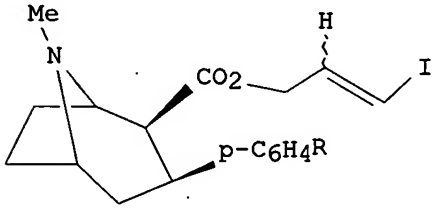
PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 136:167538

GI



I

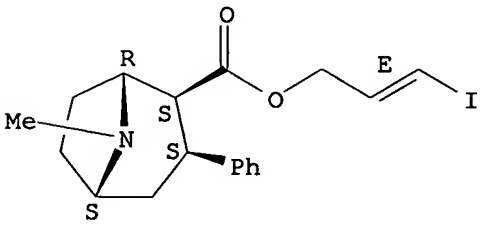
AB Tropane analogs from cocaine, which is known to be one of the most reinforcing and addictive compds., were designed, synthesized, and characterized for inhibition of presynaptic uptake of dopamine (DA) in brain. Eight new derivs. of 3β-aryl-2β-(3-iodoallyloxycarbonyl)tropanes, e.g. I ((E)-, R = H; (Z)-, R = F) were synthesized and tested for their potential abilities to displace [3H]2β-carbomethoxy-3β-(4-fluorophenyl)tropane (WIN 35,428) binding to the rat striatal membranes.

IT **396726-06-0P 396726-14-0P 396726-15-1P**
396726-16-2P 396726-17-3P 396726-18-4P
396726-19-5P 396726-20-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and binding affinities of (E)- and (Z)-2β-(3-iodoallyloxycarbonyl)-3β-aryltropane derivs. for the dopamine transporter)

RN 396726-06-0 CAPLUS

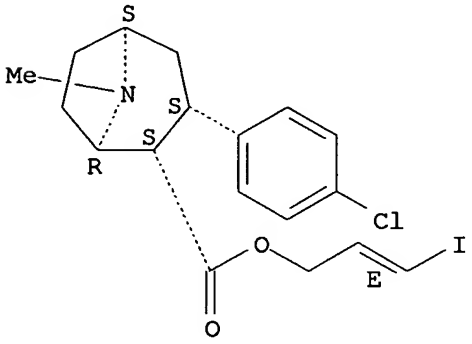
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-phenyl-, (2E)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



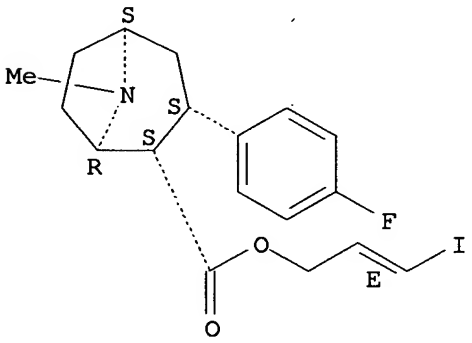
RN 396726-14-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (2E)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



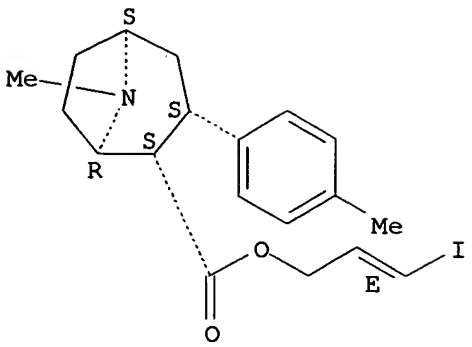
RN 396726-15-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-fluorophenyl)-8-methyl-, (2E)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



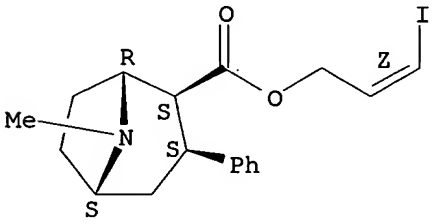
RN 396726-16-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, (2E)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



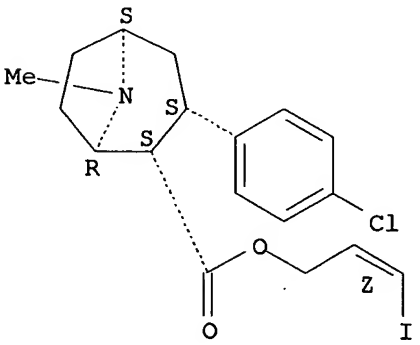
RN 396726-17-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-phenyl-, (2Z)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 396726-18-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (2Z)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

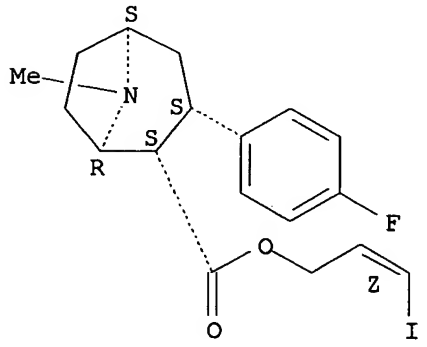
Absolute stereochemistry.
Double bond geometry as shown.



RN 396726-19-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-fluorophenyl)-8-methyl-,

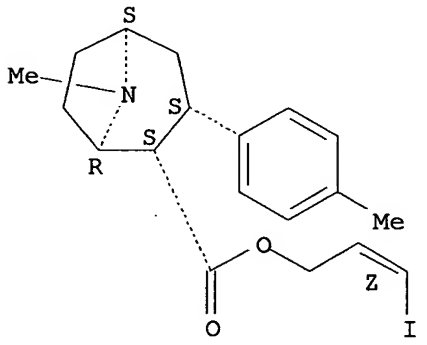
(2Z)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 396726-20-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, (2Z)-3-iodo-2-propenyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

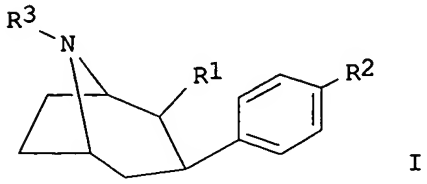
Absolute stereochemistry.
Double bond geometry as shown.



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:872201 CAPLUS
DN 136:183977
TI Synthesis and biological evaluation of a series of novel N- or O-fluoroalkyl derivatives of tropane: potential positron emission tomography (PET) imaging agents for the dopamine transporter
AU Gu, Xiao-Hui; Zong, Rushi; Kula, Nora S.; Baldessarini, Ross J.; Neumeyer, John L.
CS Medicinal Chemistry Laboratory, Alcohol and Drug Abuse Research Center, Belmont, MA, 02478-9106, USA
SO Bioorganic & Medicinal Chemistry Letters (2001), 11(23), 3049-3053
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 136:183977
GI



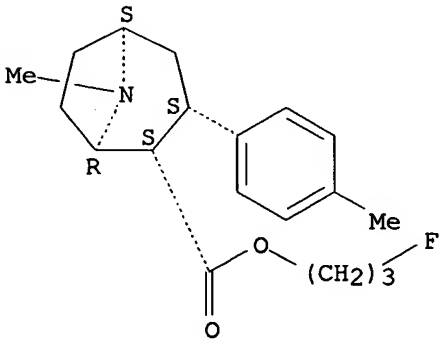
I

AB A series of novel fluoroalkyl-containing tropane derivs. was synthesized, and their binding affinities for the dopamine transporter (DAT), serotonin transporter (SERT), and norepinephrine transporter (NET) were determined via competitive binding assays. Among these derivs., the fluoropropyl ester of β-CIT (I; R1 = CO2(CH2)3F; R2 = I; R3 = Me), the fluoroethyl ester of β-CIT I (R1 = CO2(CH2)2F; R2 = I; R3 = Me), the N-fluoropropyl derivative of β-CBT I (R1 = CO2Me; R2 = Br; R3 = (CH2)3F), and the fluoropropyl ester of β-CMT I (R1 = CO2(CH2)3F; R2,R3 = Me) displayed higher affinity and greater selectivity for the DAT vs. SERT and NET than FP-CIT, which indicates that they are attractive candidates for the development of 18F-labeled PET imaging agents for the DAT.

IT **398497-77-3P 398497-79-5P 398497-81-9P 398497-84-2P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and monoamine transporter binding affinity of fluoroalkyl containing tropane derivs.)

RN 398497-77-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, 3-fluoropropyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

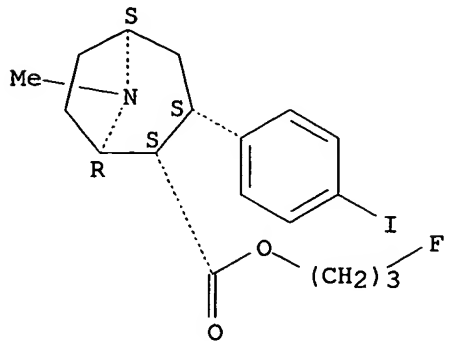
Absolute stereochemistry.



RN 398497-79-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-,

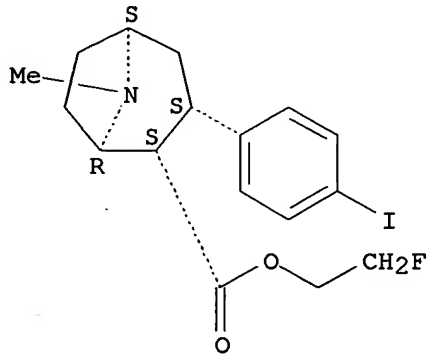
3-fluoropropyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



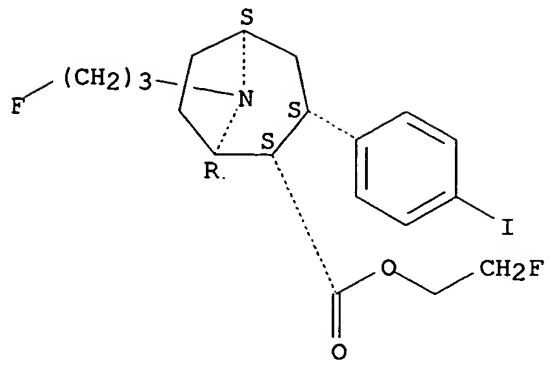
RN 398497-81-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



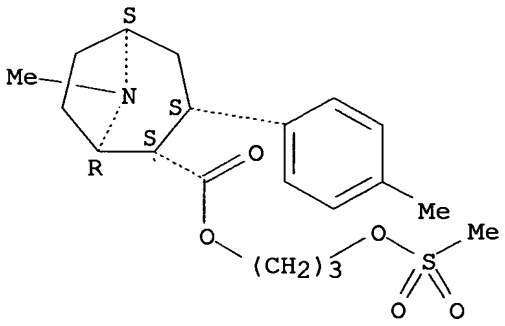
RN 398497-84-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-(3-fluoropropyl)-3-(4-iodophenyl)-, 2-fluoroethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



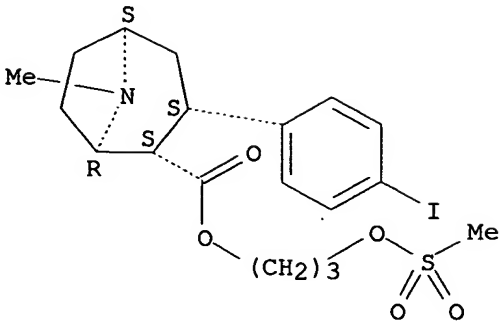
IT **398497-73-9P 398497-75-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and monoamine transporter binding affinity of fluoroalkyl containing tropane derivs.)
RN 398497-73-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, 3-[(methylsulfonyl)oxy]propyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 398497-75-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 3-[(methylsulfonyl)oxy]propyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:137949 CAPLUS
DN 135:40863
TI Biophysical characterization of the cocaine binding pocket in the serotonin transporter using a fluorescent cocaine analogue as a molecular reporter
AU Rasmussen, Soren G. F.; Carroll, F. Ivy; Maresch, Martin J.; Jensen, Anne Dam; Tate, Christopher G.; Gether, Ulrik
CS Division of Cellular and Molecular Physiology, Department of Medical Physiology, The Panum Institute, University of Copenhagen, Copenhagen N, DK-2200, Den.
SO Journal of Biological Chemistry (2001), 276(7), 4717-4723
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
AB To explore the biophys. properties of the binding site for cocaine and related compds. in the serotonin transporter SERT, a high affinity cocaine analog 3β-(4-methylphenyl)tropane-2β-carboxylic acid N-(N-methyl-N-(4-nitrobenzo-2-oxa-1,3-diazol-7-yl)ethano lamine ester hydrochloride (RTI-233); KI = 14 nM) that contained the environmentally sensitive fluorescent moiety 7-nitrobenzo-2-oxa-1,3-diazole (NBD) was synthesized. Specific binding of RTI-233 to the rat serotonin transporter, purified from Sf-9 insect cells, was demonstrated by the competitive inhibition of fluorescence using excess serotonin, citalopram, or RTI-55 (2β-carbomethoxy-3β-(4-iodophenyl)tropane). Moreover, specific binding was evidenced by measurement of steady-state fluorescence anisotropy, showing constrained mobility of bound RTI-233 relative to RTI-233 free in solution The fluorescence of bound RTI-233 displayed an emission maximum (λmax) of 532 nm, corresponding to a 4-nm blue shift as compared with the λmax of RTI-233 in aqueous solution and corresponding to the λmax of RTI-233 in 80% dioxane. Collisional quenching expts. revealed that the aqueous quencher potassium iodide was able to quench the fluorescence of RTI-233 in the binding pocket (KSV = 1.7 M-1), although not to the same extent as free RTI-233 (KSV = 7.2 M-1). Conversely, the hydrophobic quencher 2,2,6,6-tetramethylpiperidine-N-oxyl (TEMPO) quenched the fluorescence of bound RTI-233 more efficiently than free RTI-233. These data are consistent with a highly hydrophobic microenvironment in the binding pocket for cocaine-like uptake inhibitors. However, in contrast to what has been observed for small-mol. binding sites

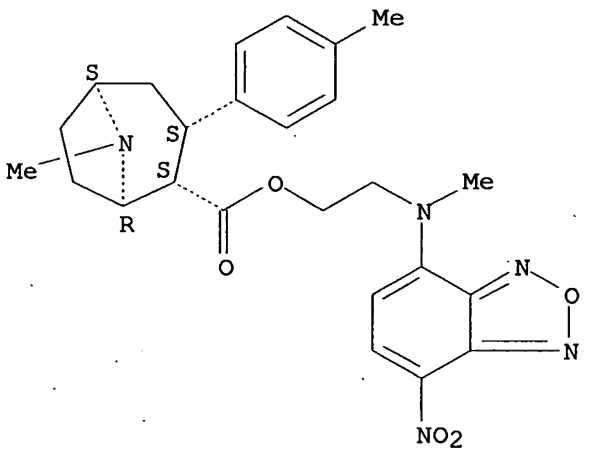
in, for example, G protein-coupled receptors, the bound cocaine analog was still accessible for aqueous quenching and, thus, partially exposed to solvent.

IT **344606-91-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(biophys. characterization of the cocaine binding pocket in the serotonin transporter using a fluorescent cocaine analog as a mol. reporter)

RN 344606-91-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, 2-[methyl(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]ethyl ester, monohydrochloride, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:68946 CAPLUS

DN 132:251272

TI Synthesis, Biodistribution, and Primate Imaging of Fluorine-18 Labeled 2β-Carbo-1'-fluoro-2-propoxy-3β-(4-chlorophenyl)tropanes. Ligands for the Imaging of Dopamine Transporters by Positron Emission Tomography

AU Xing, Dongxia; Chen, Ping; Keil, Robert; Kilts, Clinton D.; Shi, Bing; Camp, Vernon M.; Malveaux, Gene; Ely, Timothy; Owens, Michael J.; Votaw, John; Davis, Margaret; Hoffman, John M.; BaKay, Roy A. E.; Subramanian, Thygarajan; Watts, Ray L.; Goodman, Mark M.

CS Emory Center for Positron Emission Tomography and Departments of Radiology Psychiatry and Behavior Sciences Neurology and Neurosurgery, Emory University, Atlanta, GA, 30320, USA

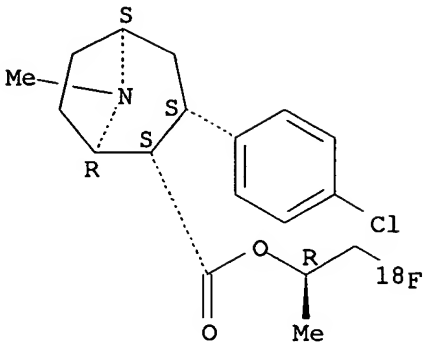
SO Journal of Medicinal Chemistry (2000), 43(4), 639-648

CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB 2β-(R)-Carbo-1-fluoro-2-propoxy-3β-(4-chlorophenyl)tropane ((R)-FIPCT) and 2β-(S)-carbo-1-fluoro-2-propoxy-3β-(4-chlorophenyl)tropane ((S)-FIPCT) were prepared and evaluated in vitro and in vivo for dopamine transporter (DAT) selectivity and specificity. High specific activity [18F](R)-FIPCT and [18F](S)-FIPCT were synthesized in 5% radiochem. yield (decay-corrected to end of bombardment (EOB)) by preparation of the precursors 2β-carbo-R-1-mesyloxy-2-propoxy-3β-(4-chlorophenyl)tropane and 2β-carbo-S-1-mesyloxy-2-propoxy-3β-(4-chlorophenyl)tropane followed by treatment with no carrier-added potassium[18F]fluoride and kyrptofix K222 in acetonitrile. Competition binding in cells stably expressing the transfected human DAT and serotonin transporter (SERT) labeled by [3H]WIN 35428 and [3H]citalopram, resp., demonstrated the following order of DAT affinity (Ki in nM): GBR 12909 (0.36) > CIT (0.48) > (S)-FIPCT (0.67) » (R)-FIPCT (3.2). The affinity of (S)-FIPCT and (R)-FIPCT for SERT was 127- and 20-fold lower, resp., than for DAT. In vivo biodistribution studies were performed in male rats and demonstrated that the brain uptake of [18F](R)-FIPCT and [18F](S)-FIPCT were selective and specific for DAT rich regions (caudate and putamen). PET brain imaging studies in monkeys demonstrated high [18F](R)-FIPCT and [18F](S)-FIPCT uptake in the caudate and putamen which resulted in caudate-to-cerebellum and putamen-to-cerebellum ratios of 2.5-3.5 at 115 min. [18F](R)-FIPCT uptake in the caudate/putamen achieved transient equilibrium at 75 min. In an imaging experiment with [18F](S)-FIPCT in a rhesus monkey with its left hemisphere lesioned with MPTP, radioactivity was reduced to background in the caudate and putamen of the lesioned hemisphere. The high specific activity one-step radiolabeling preparation and high specificity and selectivity of [18F](R)-FIPCT and [18F](S)-FIPCT for DAT indicate [18F](R)-FIPCT and [18F](S)-FIPCT are potential radioligands for mapping brain DAT in humans using PET.

IT **262423-87-0P 262423-88-1P 262423-89-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, biodistribution, and primate imaging of fluorine-18 labeled 2β-carbo-1'-fluoro-2-propoxy-3β-(4-chlorophenyl)tropanes, ligands for imaging of dopamine transporters by positron emission tomog.)

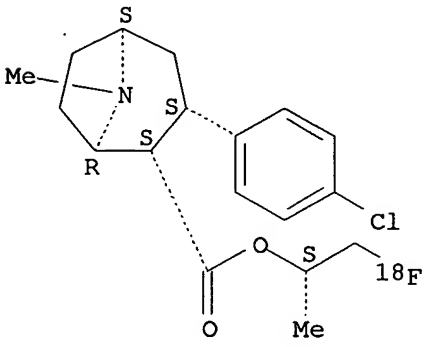
RN 262423-87-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (1R)-2-(fluoro-18F)-1-methylethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



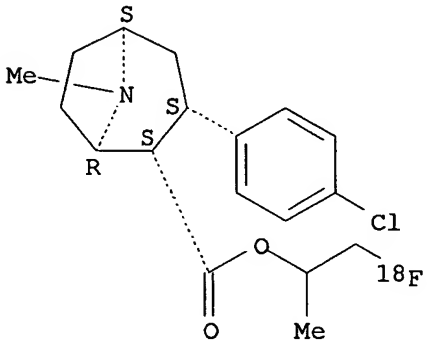
RN 262423-88-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (1S)-2-(fluoro-18F)-1-methylethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 262423-89-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, 2-(fluoro-18F)-1-methylethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

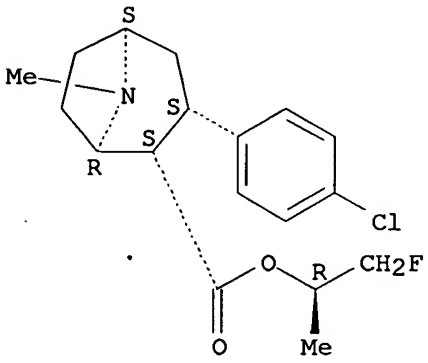
Absolute stereochemistry.



IT **262423-85-8P 262423-86-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis, biodistribution, and primate imaging of fluorine-18 labeled 2β-carbo-1'-fluoro-2-propoxy-3β-(4-chlorophenyl)tropanes, ligands for imaging of dopamine transporters by positron emission tomog.)

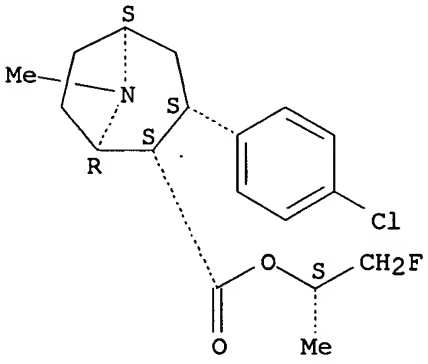
RN 262423-85-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (1R)-2-fluoro-1-methylethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 262423-86-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (1S)-2-fluoro-1-methylethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

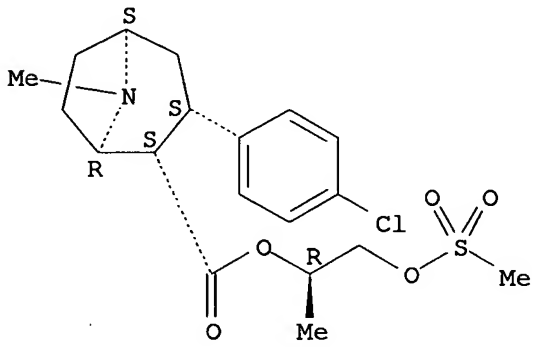
Absolute stereochemistry.



IT **262423-82-5P 262423-84-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis, biodistribution, and primate imaging of fluorine-18 labeled 2β-carbo-1'-fluoro-2-propoxy-3β-(4-chlorophenyl)tropanes, ligands for imaging of dopamine transporters by positron emission

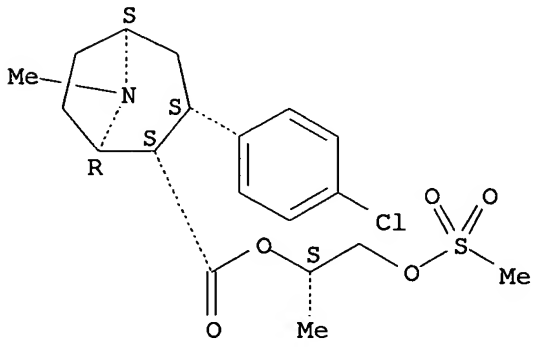
tomog.)
RN 262423-82-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (1R)-1-methyl-2-[(methylsulfonyl)oxy]ethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



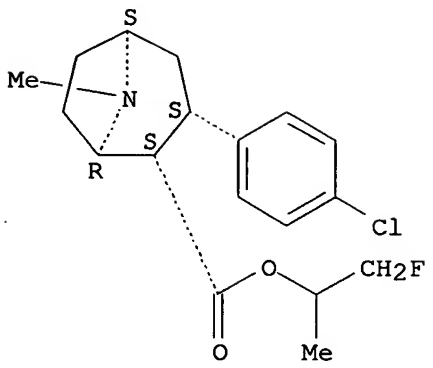
RN 262423-84-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, (1S)-1-methyl-2-[(methylsulfonyl)oxy]ethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **262423-80-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis, biodistribution, and primate imaging of fluorine-18 labeled 2β-carbo-1'-fluoro-2-propoxy-3β-(4-chlorophenyl)tropanes, ligands for imaging of dopamine transporters by positron emission tomog.)
RN 262423-80-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, 2-fluoro-1-methylethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



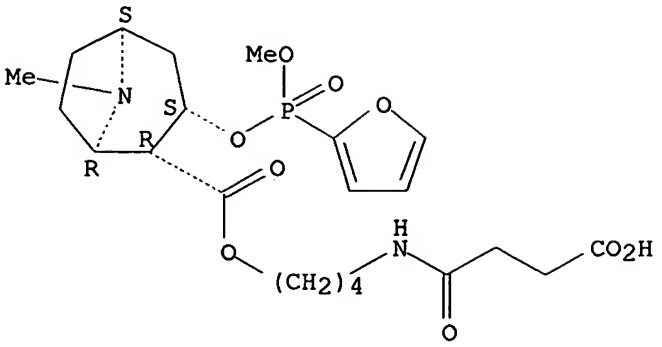
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:705039 CAPLUS
DN 131:318871
TI Catalytic antibodies against cocaine
IN Landry, Donald W.; Zhao, Kang
PA The Trustees of Columbia University in the City of New York, USA
SO U.S., 39 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5977314	A	19991102	US 1995-477300	19950607
PRAI US 1995-477300		19950607		

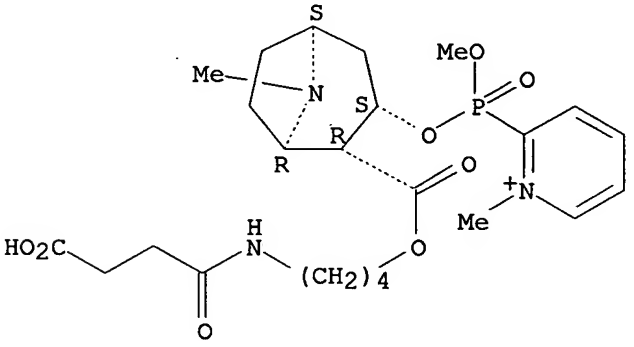
OS MARPAT 131:318871
AB This invention provides compds. which are analogs to the hydrolysis transition-state of a cocaine benzoyl ester group. This invention also provides such analogs linked to carrier proteins, and antibodies thereto. This invention further provides pharmaceutical composition for decreasing concentration in a subject using the antibodies produced.
IT **248959-66-2D**, adduct with carrier protein **248959-67-3D**, adduct with carrier protein **248959-69-5D**, adduct with carrier protein **248959-70-8D**, adduct with carrier protein
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of antibodies and catalytic antibodies against cocaine)
RN 248959-66-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(2-furanylmethoxyphosphinyl)oxy]-8-methyl-, 4-[(3-carboxy-1-oxopropyl)amino]butyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



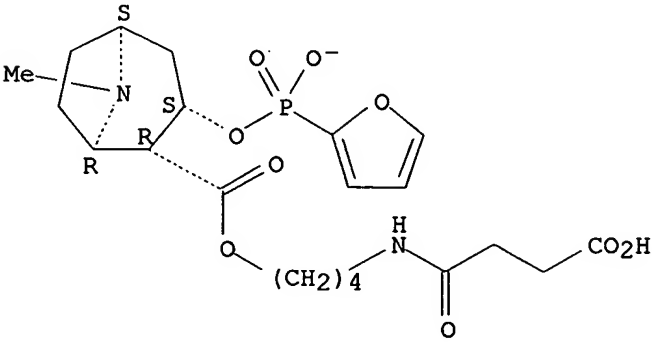
RN 248959-67-3 CAPLUS
CN Pyridinium, 2-[[[(1R,2R,3S,5S)-2-[[4-[(3-carboxy-1-oxopropyl)amino]butoxy]carbonyl]-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]oxy]methoxyphosphinyl]-1-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



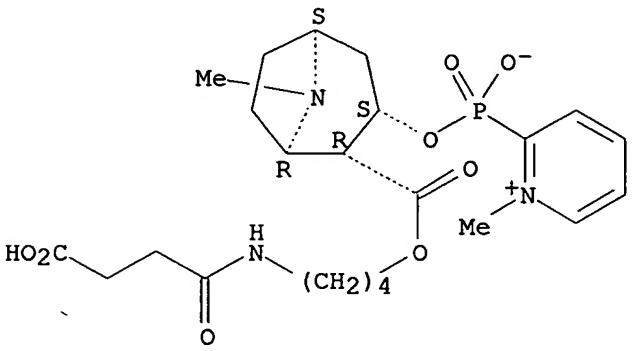
RN 248959-69-5 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(2-furanylhydroxyphosphinyl)oxy]-8-methyl-, 4-[(3-carboxy-1-oxopropyl)amino]butyl ester, ion(1-), (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



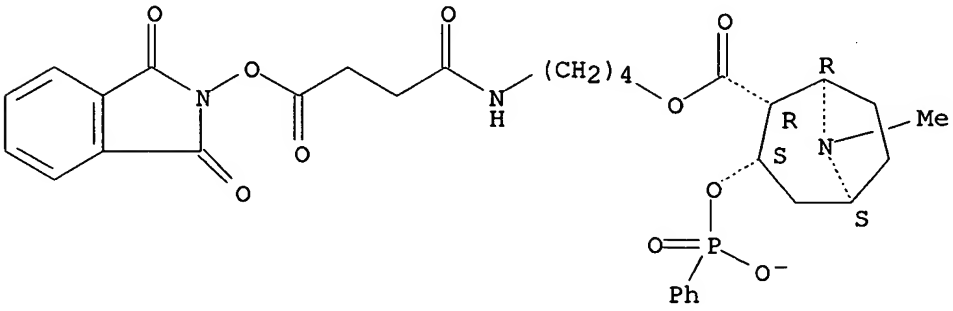
RN 248959-70-8 CAPLUS
CN Pyridinium, 2-[[[(1R,2R,3S,5S)-2-[[4-[(3-carboxy-1-oxopropyl)amino]butoxy]carbonyl]-8-methyl-8-azabicyclo[3.2.1]oct-3-yl]oxy]hydroxyphosphinyl]-1-methyl-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **248959-64-0DP**, reaction products with primary amines of carrier protein
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of antibodies and catalytic antibodies against cocaine)
RN 248959-64-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(hydroxyphenylphosphinyl)oxy]-8-methyl-, 4-[[4-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)oxy]-1,4-dioxobutyl]amino]butyl ester, ion(1-), (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

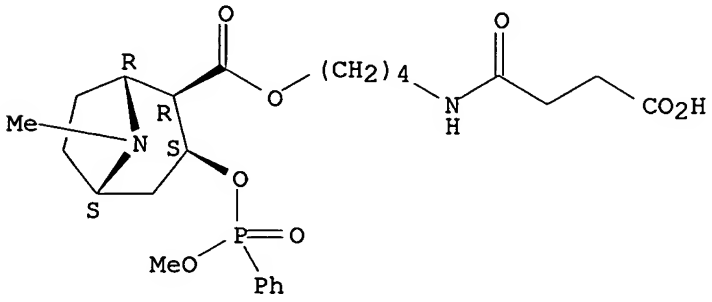
Absolute stereochemistry.



IT **152241-57-1P 152241-60-6P 152241-61-7P 152241-62-8P 248959-63-9P 248959-64-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of antibodies and catalytic antibodies against cocaine)
RN 152241-57-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-

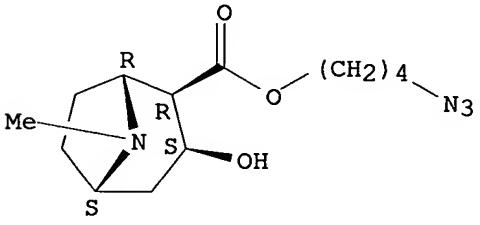
[(methoxyphenylphosphinyl)oxy]-8-methyl-, 4-[(3-carboxy-1-oxopropyl)amino]butyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



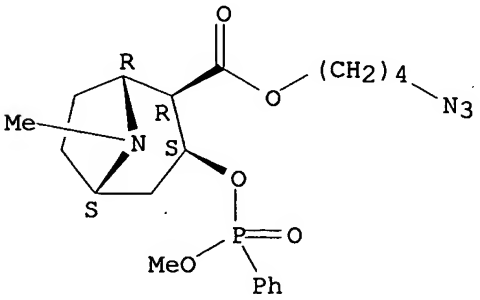
RN 152241-60-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 4-azidobutyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 152241-61-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(methoxyphenylphosphinyl)oxy]-8-methyl-, 4-azidobutyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

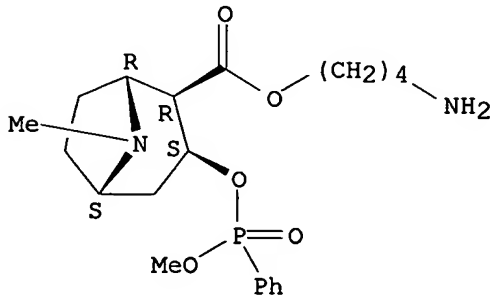
Absolute stereochemistry.



RN 152241-62-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-

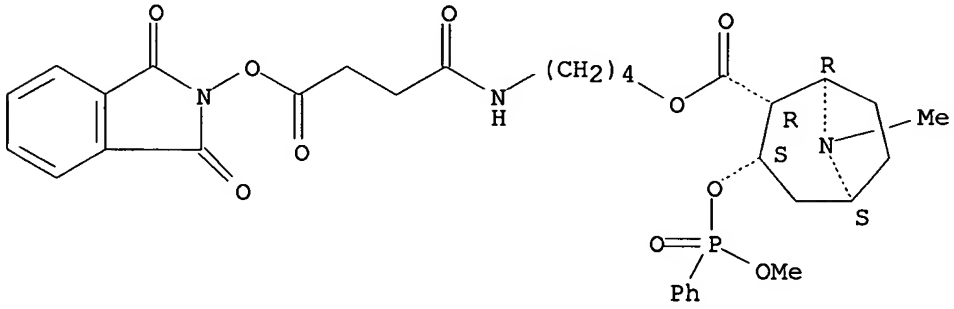
[(methoxyphenylphosphinyl)oxy]-8-methyl-, 4-aminobutyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



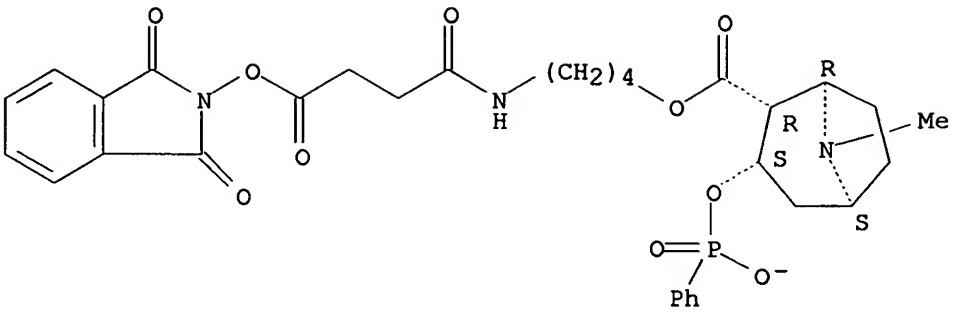
RN 248959-63-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(methoxyphenylphosphinyl)oxy]-8-methyl-, 4-[[4-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)oxy]-1,4-dioxobutyl]amino]butyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 248959-64-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(hydroxyphenylphosphinyl)oxy]-8-methyl-, 4-[[4-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)oxy]-1,4-dioxobutyl]amino]butyl ester, ion(1-), (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

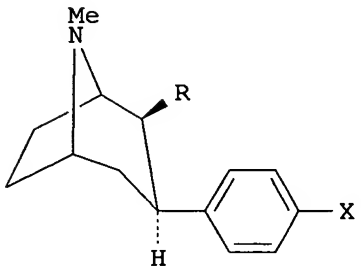


RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:505661 CAPLUS
DN 131:157708
TI Methods for controlling invertebrate pests using cocaine receptor binding ligands
IN Kuhar, Michael J.; Carroll, Frank I.; Boja, John W.; Lewin, Anita H.; Abraham, Philip
PA Research Triangle Institute, USA
SO U.S., 58 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 12

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5935953	A	19990810	US 1997-823563	19970325
	US 564755	A0	19910801	US 1990-564755	19900809
	US 5128118	A	19920707		
	US 5413779	A	19950509	US 1993-972472	19930323
	US 5736123	A	19980407	US 1995-436970	19950508
	US 6531483	B1	20030311	US 1996-706263	19960904
	CA 2263961	AA	19980226	CA 1997-2263961	19970822
	WO 9807427	A1	19980226	WO 1997-US14702	19970822
	W: AU, CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9742327	A1	19980306	AU 1997-42327	19970822
	EP 993301	A1	20000419	EP 1997-940580	19970822
	EP 993301	B1	20030409		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2001525795	T2	20011211	JP 1998-510955	19970822
	AT 236635	E	20030415	AT 1997-940580	19970822
PRAI	US 1990-564755	A2	19900809		
	US 1993-972472	A2	19930323		
	US 1995-436970	A2	19950508		
	US 1995-506541	A2	19950724		
	US 1996-701503	A2	19960822		
	US 1996-706263	A2	19960904		
	WO 1991-US5553	W	19910809		
	US 1991-792648	B2	19911115		

US 1993-164576 A2 19931210
US 1997-823563 A 19970325
WO 1997-US14702 W 19970822
OS MARPAT 131:157708
GI



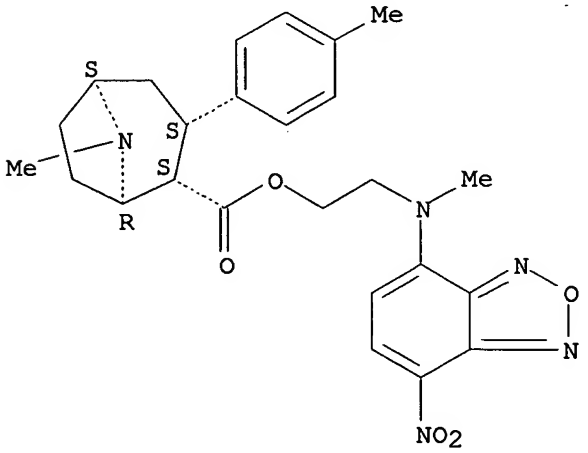
I

AB Tropane derivs. such as I (R = heterocyclyl; X = Cl, Me) were prepared as inhibitors of a phenylethanolamine reuptake transporter in invertebrate pests. Thus, refluxing 2 mmol 3β-(4-chlorophenyl)tropane-2β-carboxylic acid in 2 mL POCl3 with 2.2 mmol benzoic acid hydrazide 2 h gave a 42% yield of I (R = 5-phenyl-1,3,4-oxadiazol-2-yl, X = Cl). The IC50 values at dopamine, serotonin, and norepinephrine receptors were determined

IT **236753-85-8**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(controlling invertebrate pests by using cocaine receptor binding ligands)

RN 236753-85-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, 2-[methyl(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]ethyl ester, (1R,2S,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

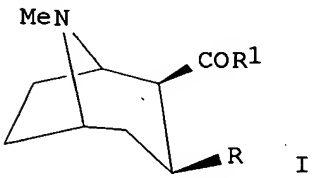


RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:253997 CAPLUS
DN 126:238537
TI Preparation of labeled cocaine analogs
IN Goodman, Mark M.; Shi, Bing Zhi; Keil, Robert N.
PA Emory University, USA; Goodman, Mark M.; Shi, Bing Zhi; Keil, Robert N.
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9706832	A1	19970227	WO 1996-US13471	19960812
	W: AU, CA, JP, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 5864038	A	19990126	US 1995-512516	19950817
	AU 9672348	A1	19970312	AU 1996-72348	19960812
	US 5888475	A	19990330	US 1997-948791	19971010
PRAI	US 1995-512516	A	19950817		
	WO 1996-US13471	W	19960812		

OS MARPAT 126:238537
GI



I

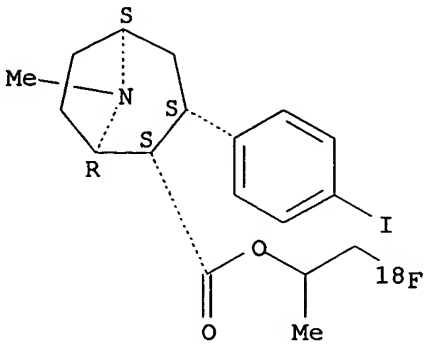
AB The labeled cocaine analogs I (R = Ph, naphthyl, iodo or trimethylsilyl substituted Ph or naphthyl; R1 = fluoroalkoxy, methanesulfonyloxyalkoxy; the iodo or fluoro may be radio-labeled) were prepared as agents useful for diagnostic imaging of the brain, in particular those regions having dopaminergic neurons. Such imaging is useful for differential diagnosis of Parkinson's disease and for the monitoring of addictive disorders related to abuse of cocaine and treatment thereof. Thus, I (R = 4-IC6H4, R1 = CO2CHMeCH2O3SMe), prepared in 4 steps from (-)-anhydroecoginie Me ester, was treated with treated with K18F to give I (R = 4-IC6H4, R1 = CO2CHMeCH218F) (II). The distribution of radioactivity in tissues of unfasted Sprague Dawley rats following i.v. administration of II was determined

IT **188425-12-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of labeled cocaine analogs as imaging agents)

RN 188425-12-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-,

2-(fluoro-18F)-1-methylethyl ester, [1R-(1α,2α,3α,5.alph
a.)]-[partial]- (9CI) (CA INDEX NAME)

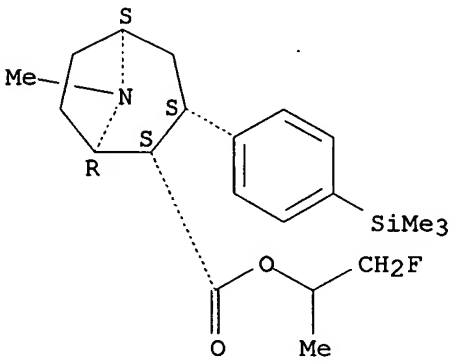
Absolute stereochemistry.



IT **188425-13-0P 188425-14-1P 188425-15-2P**
188425-17-4P 188425-22-1P 188425-23-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of labeled cocaine analogs as imaging agents)

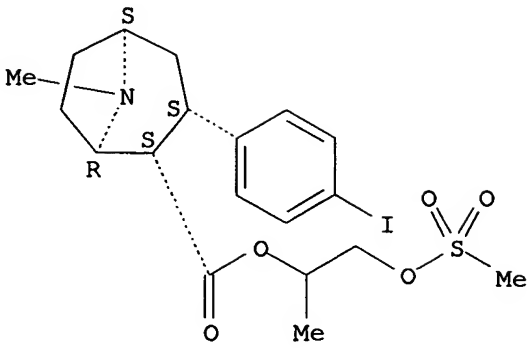
RN 188425-13-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-[4-(trimethylsilyl)phenyl]-, 2-fluoro-1-methylethyl ester, [1R-(1α,2α,3α,5α)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



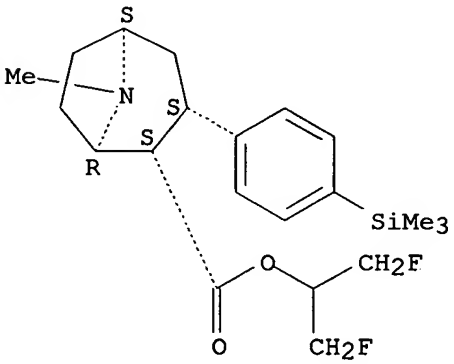
RN 188425-14-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 1-methyl-2-[(methylsulfonyl)oxy]ethyl ester, [1R-(1α,2α,3α,5α)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



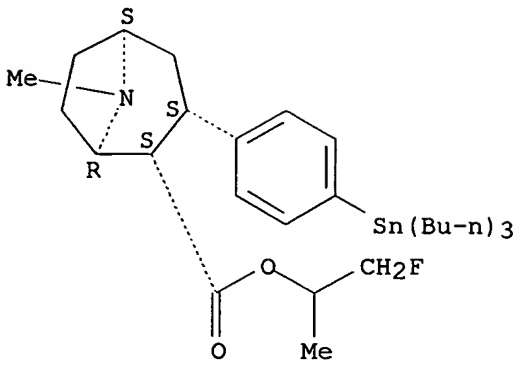
RN 188425-15-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-[4-(trimethylsilyl)phenyl]-, 2-fluoro-1-(fluoromethyl)ethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



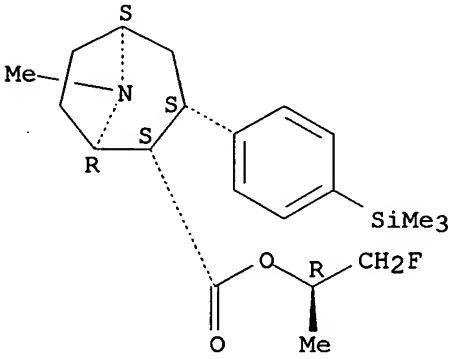
RN 188425-17-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-[4-(tributylstannyl)phenyl]-, 2-fluoro-1-methylethyl ester, [1R-(1α,2α,3α,5α)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



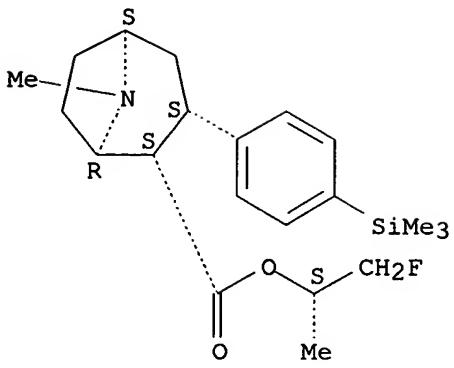
RN 188425-22-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-[4-(trimethylsilyl)phenyl]-, 2-fluoro-1-methylethyl ester, [1R-[1α,2α(R*),3α,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 188425-23-2 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-[4-(trimethylsilyl)phenyl]-, 2-fluoro-1-methylethyl ester, [1R-[1α,2α(S*),3α,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

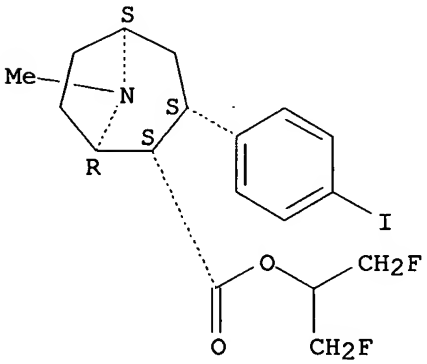


IT **188425-16-3P 188425-18-5P 188425-19-6P**
188425-20-9P 188425-21-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of labeled cocaine analogs as imaging agents)

RN 188425-16-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-fluoro-1-(fluoromethyl)ethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

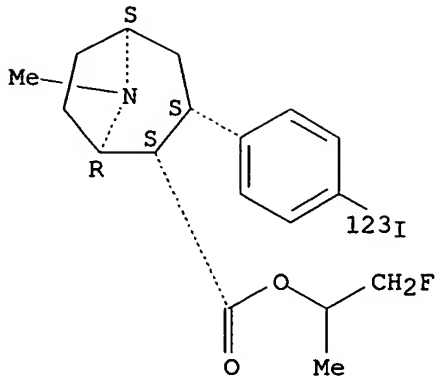
Absolute stereochemistry.



RN 188425-18-5 CAPLUS

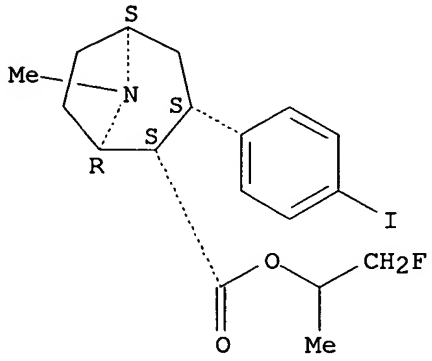
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[4-(iodo-123I)phenyl]-8-methyl-, 2-fluoro-1-methylethyl ester, [1R-(1α,2α,3α,5.alpha.)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



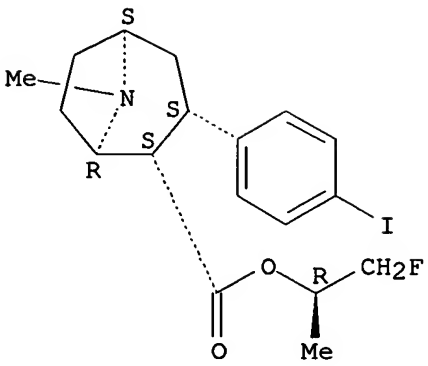
RN 188425-19-6 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-fluoro-1-methylethyl ester, [1R-(1α,2α,3α,5α)]- [partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



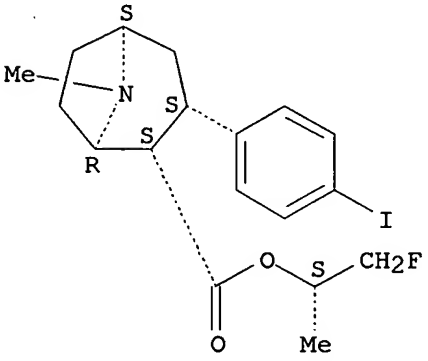
RN 188425-20-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-fluoro-1-methylethyl ester, [1R-[1α,2α(R*),3α,5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

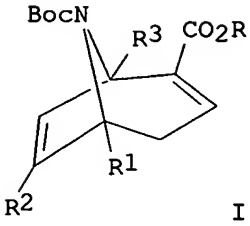


RN 188425-21-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-iodophenyl)-8-methyl-, 2-fluoro-1-methylethyl ester, [1R-[1α,2α(S*),3α,5α]]- (9CI) (CA INDEX NAME)

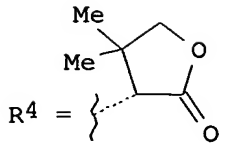
Absolute stereochemistry.



L5 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:88844 CAPLUS
DN 126:171751
TI Enantioselective Synthesis of Functionalized Tropanes by Rhodium(II) Carboxylate-Catalyzed Decomposition of Vinyldiazomethanes in the Presence of Pyrroles
AU Davies, Huw M. L.; Matasi, Julius J.; Hodges, L. Mark; Huby, Nicholas J. S.; Thornley, Craig; Kong, Norman; Houser, Jeffrey H.
CS Department of Chemistry, State University of New York at Buffalo Buffalo, Buffalo, NY, 14260-3000, USA
SO Journal of Organic Chemistry (1997), 62(4), 1095-1105
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 126:171751
GI



I



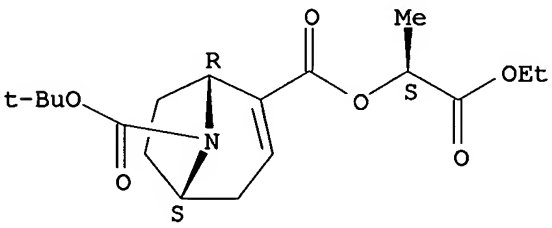
AB A series of enantiomerically enriched tropanes, e.g. I [R = CHMeCO2Et-(S), R1-R3 = H; R1 = Me, CH2OSiMe2CMe3, Ph, Ac, R2 = R3 = H; R1 = R3 = Me, R2 = H; R1 = R3 = H, R2 = Me; R1R2 = (CH2)4, R3 = H; R = R4, R1-R3 = H], was synthesized by the rhodium(II) octanoate-catalyzed reaction of various N-BOC-protected pyrroles with vinyldiazomethanes. The overall [3 + 4]-annulation occurs by a tandem cyclopropanation/Cope rearrangement. Asym. induction was best achieved in these transformations by using either (S)-lactate or (R)-pantolactone as a chiral auxiliary on the vinyldiazomethanes. Reactions carried out with the chiral catalyst tetrakis[N-(4-tert-butylbenzenesulfonyl)-L-prolinato]dirhodium provided moderate asym. induction, but also resulted in the formation of isomeric azabicyclooctane side products. The utility of the synthetic process was demonstrated through the asym. synthesis of (-)-anhydroecgonine Me ester and (-)-ferruginine.

IT **186898-85-1P 186898-91-9P 186899-10-5P 186899-18-3P 186899-19-4P 186899-20-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of tropane alkaloids by rhodium carboxylate-catalyzed cycloaddns. of vinyldiazomethanes with pyrroles)

RN 186898-85-1 CAPLUS

CN 8-Azabicyclo[3.2.1]oct-2-ene-2,8-dicarboxylic acid, 8-(1,1-dimethylethyl) 2-(2-ethoxy-1-methyl-2-oxoethyl) ester, [1R-[1α,2(S*),5α]]- (9CI) (CA INDEX NAME)

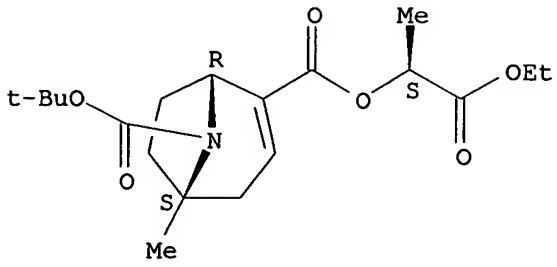
Absolute stereochemistry.



RN 186898-91-9 CAPLUS

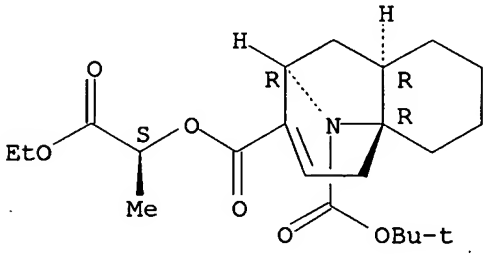
CN 8-Azabicyclo[3.2.1]oct-2-ene-2,8-dicarboxylic acid, 5-methyl-, 8-(1,1-dimethylethyl) 2-(2-ethoxy-1-methyl-2-oxoethyl) ester, [1R-[1α,2(S*),5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



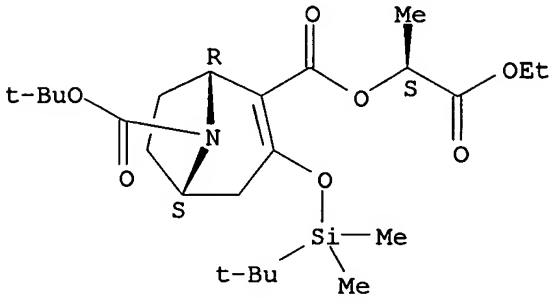
RN 186899-10-5 CAPLUS
CN 4aH-Benzocyclohepten-4a,8-imine-7,10-dicarboxylic acid, 1,2,3,4,5,8,9,9a-octahydro-, 10-(1,1-dimethylethyl) 7-(2-ethoxy-1-methyl-2-oxoethyl) ester, [4aR-[4aα,7(S*),8α,9aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 186899-18-3 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2,8-dicarboxylic acid, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, 8-(1,1-dimethylethyl) 2-(2-ethoxy-1-methyl-2-oxoethyl) ester, [1R-[1α,2(S*),5α]]- (9CI) (CA INDEX NAME)

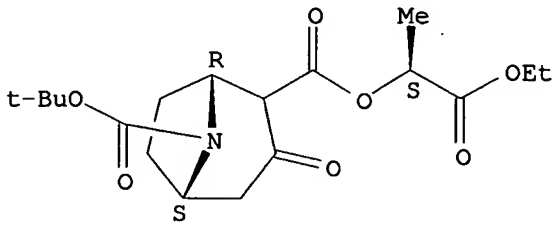
Absolute stereochemistry.



RN 186899-19-4 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2,8-dicarboxylic acid, 3-oxo-,

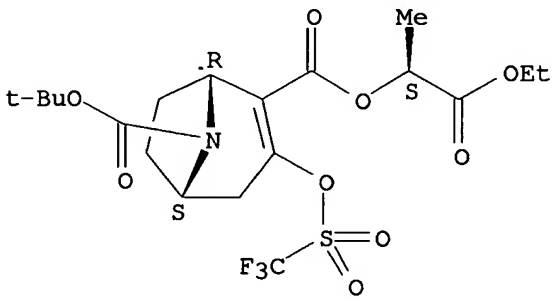
8-(1,1-dimethylethyl) 2-(2-ethoxy-1-methyl-2-oxoethyl) ester, [1R,2(S),5S]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



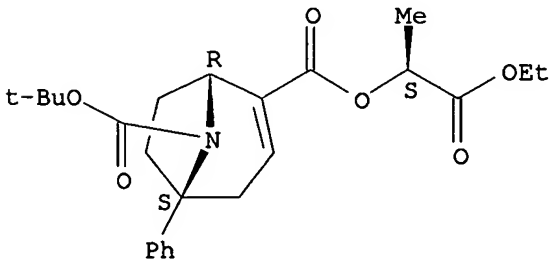
RN 186899-20-7 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2,8-dicarboxylic acid, 3-[[(trifluoromethyl)sulfonyl]oxy]-, 8-(1,1-dimethylethyl) 2-(2-ethoxy-1-methyl-2-oxoethyl) ester, [1R-[1α,2(S*),5α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **186899-09-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of tropane alkaloids by rhodium carboxylate-catalyzed cycloaddns. of vinyldiazomethanes with pyrroles)
RN 186899-09-2 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2,8-dicarboxylic acid, 5-phenyl-, 8-(1,1-dimethylethyl) 2-(2-ethoxy-1-methyl-2-oxoethyl) ester, [1R-[1α,2(S*),5α]]- (9CI) (CA INDEX NAME)

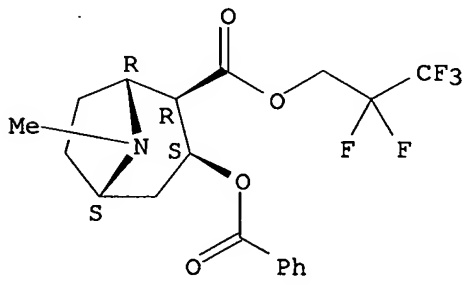
Absolute stereochemistry.



RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

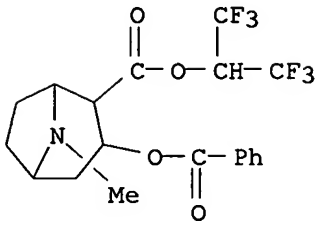
L5 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:599890 CAPLUS
DN 125:294843
TI One-step esterification of benzoylecgonine with dimethylformamide-dipropylacetal or dimethylformamide-diisopropylacetal in the presence of pyridine
AU Paul, Buddha D.; Dreka, Catherine; Summers, Jacqueline L.; Smith, Michael L.
CS Division Forensic Toxicology, Office Armed Forces Medical Examiner, Armed Forces Institute Pathology, Rockville, MD, 20706, USA
SO Journal of Analytical Toxicology (1996), 20(6), 506-508
CODEN: JATOD3; ISSN: 0146-4760
PB Preston Publications
DT Journal
LA English
AB A simple procedure was developed to derivatize benzoylecgonine extracted from urine for subsequent confirmation by gas chromatog.-mass spectrometry. The compound was esterified with dimethylformamide-dipropylacetal (DMF-DPA) or dimethylformamide-diisopropylacetal (DMF-DIPA) to the corresponding Pr and iso-Pr esters. The optimum reaction condition was found to be heating the reaction mixture in the presence of pyridine at 100°C for 30 min. The procedure is a one-step esterification followed by evaporation of excess reagents. When benzoylecgonine was extracted from urine using a solid-phase extraction technique and derivatized with this procedure, the compound was detected at a level as low as 10 ng/mL. Quantitation was linear over the concentration range 10-8000 ng/mL.
IT **128429-28-7 182759-76-8**
RL: ANT (Analyte); ANST (Analytical study)
(esterification of benzoylecgonine with dimethylformamide-dipropylacetal or dimethylformamide-diisopropylacetal in the presence of pyridine)
RN 128429-28-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2,2,3,3,3-pentafluoropropyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



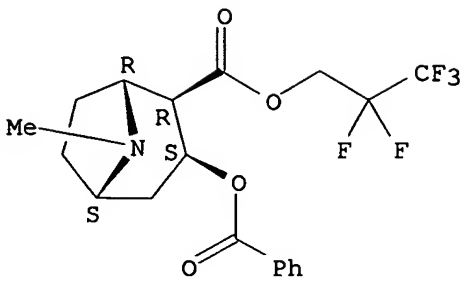
RN 182759-76-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2,2,2-trifluoro-1-(trifluoromethyl)ethyl ester, [1R-(exo,exo)]- (9CI) (CA

INDEX NAME)



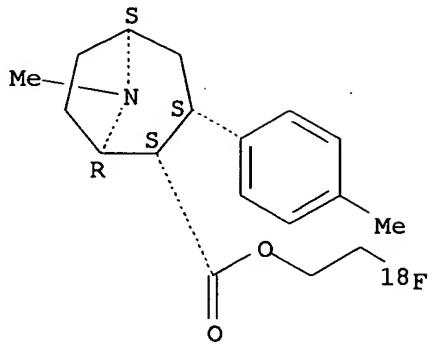
L5 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:389079 CAPLUS
DN 125:78734
TI Elimination of fluconazole interference in gas chromatography/mass spectrometric confirmation of benzoylecgonine, the major metabolite of cocaine using pentafluoropropionyl derivative
AU Dasgupta, Amitava; Mahle, Christina; McLemore, Jerri
CS Health Sciences Center, University New Mexico, Albuquerque, NM, USA
SO Journal of Forensic Sciences (1996), 41(3), 511-513
CODEN: JFSCAS; ISSN: 0022-1198
PB American Society for Testing and Materials
DT Journal
LA English
AB Cocaine is a widely abused drug and causes death from overdose. Benzoylecgonine, the major metabolite of cocaine in urine is usually confirmed after derivatization by gas chromatog./mass spectrometry to demonstrate cocaine abuse. Recently, Wu et al. demonstrated that fluconazole coelutes with benzoylecgonine after conversion to trimethylsilyl analogs and causes false-neg. result in the confirmation test. However, fluconazole did not interfere with the screening assay using an enzyme multiplied immunoassay technique. We demonstrated that by converting benzoylecgonine to the corresponding pentafluoropropionyl derivative, the interference of fluconazole can be completely eliminated. The pentafluoropropionyl derivative of benzoylecgonine eluted at 14.7 min while the derivatized fluconazole eluted at 15.6 min. The mass spectral fragmentation pattern of derivatized benzoylecgonine was distinctively different from the mass spectral features of derivatized fluconazole in both electron ionization and chemical ionization mode of operation of mass spectrometers. The quantitation of benzoylecgonine in pos. urine specimens was not affected when the specimens were supplemented with 50 μg/mL of fluconazole.
IT **128429-28-7**
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(fluconazole interference in GC/MS confirmation of benzoylecgonine)
RN 128429-28-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2,2,3,3,3-pentafluoropropyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



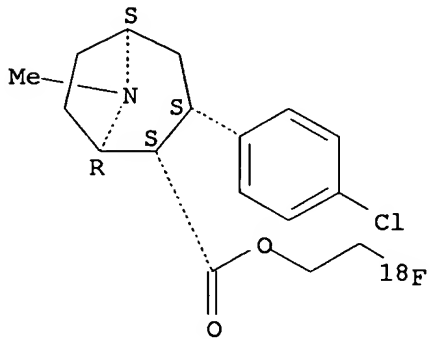
L5 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:224930 CAPLUS
DN 124:311292
TI In vivo evaluation of [11C]- and [18F]-labeled cocaine analogs as potential dopamine transporter ligands for positron emission tomography
AU Wilson, Alan A.; DaSilva, Jean N.; Houle, Sylvain
CS FACULTY MEDICINE, UNIVERSITY TORONTO, Toronto, ON, M5T 1R8, Can.
SO Nuclear Medicine and Biology (1996), 23(2), 141-6
CODEN: NMBIEO; ISSN: 0883-2897
PB Elsevier
DT Journal
LA English
AB Four analogs of the potent dopamine transporter ligand, WIN 35,428, were radiolabeled with 11C and 18F at the 2-β-carboxy position for evaluation as potential ligands for imaging dopamine uptake sites by positron emission tomog. (PET) namely, Me (1R-2-exo-3-exo)-8-methyl-3-(4-methylphenyl)-8-azabicyclo[3.2.1]octane-2-carboxylate (RTI-32), its 4-chlorophenyl analog (RTI-31), 2'-fluoroethyl (1R-2-exo-3-exo)-8-methyl-3-(4-methylphenyl)-8-azabicyclo[3.2.1]octane-2-carboxylate (FETT) and its 4-chlorophenyl analog (FECT). Upon i.v. injection in rats, all four radiotracers displayed preferential accumulation of radioactivity in regions known to contain high concns. of dopamine uptake sites. Competition studies with two of the analogs, [11C]RTI-32 and [18F]FETT, demonstrated that, for both radiotracers, binding was saturable and displayed the appropriate pharmacol. as potential PET ligands for imaging the dopamine transporter. Striatum to cerebellar ratios for [11C]RTI-32 (at 90 min post-injection) and [18F]FETT (at 120 min post-injection) were 27 and 21, resp.
IT **170163-94-7 170163-95-8**
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
([11C]- and [18F]-labeled cocaine analogs in vivo evaluation for potential PET of dopamine transporter in brain)
RN 170163-94-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, 2-(fluoro-18F)ethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 170163-95-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, 2-(fluoro-18F)ethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:1004551 CAPLUS
DN 124:135375
TI Suppression of psychoactive effects of cocaine by active immunization
AU Carrera, M. Rocio A.; Ashley, Jon A.; Parsons, Loren H.; Wirsching, Peter; Koob, George F.; Janda, Kim D.
CS Dep. Neuropharmacology Dep. Mol. Biol. Chem., Scripps Res. Inst., La Jolla, CA, 92037, USA
SO Nature (London) (1995), 378(6558), 727-30
CODEN: NATUAS; ISSN: 0028-0836
PB Macmillan Magazines
DT Journal
LA English
AB Cocaine is a powerfully addictive substance and new strategies are needed to treat its abuse. Generating an active immunization to cocaine offers a means of blocking the actions of the drug by preventing it from entering the central nervous system, and should have fewer side effects than treatments based on manipulation of central neurotransmitter function. The design and preparation of a cocaine immunogen requires special regard for the stability of cocaine both free and as a haptenic determinant.

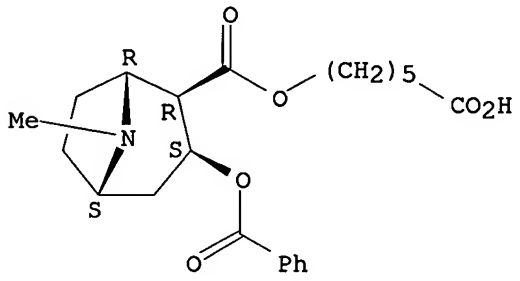
Immunochem. and a well defined behavioral model were brought together to address the problem of inactivation of the psychostimulant actions of cocaine. The authors report here that active immunization with a new, stable cocaine conjugate suppressed locomotor activity and stereotyped behavior in rats induced by cocaine but not by amphetamine. Moreover, following acute injection of cocaine, levels of cocaine in the striatum and cerebellum of the immunized animals were lower than those of control animals. These results suggest that immunopharmacotherapy may be a promising means by which to explore new treatments for cocaine abuse.

IT **173443-27-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(conjugates with keyhole limpet hemocyanin, immunization with; suppression of psychoactive effects of cocaine and brain levels by active immunization with cocaine immunoconjugate)

RN 173443-27-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 5-carboxypentyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

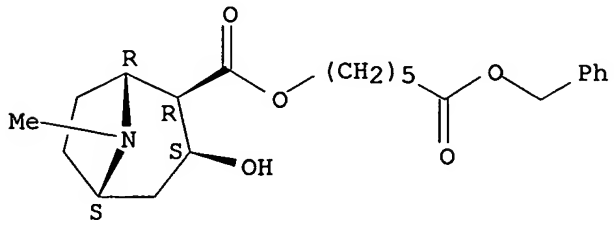


IT **173443-25-9P 173443-26-0P 173443-27-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; suppression of psychoactive effects of cocaine and brain levels by active immunization with cocaine immunoconjugate)

RN 173443-25-9 CAPLUS

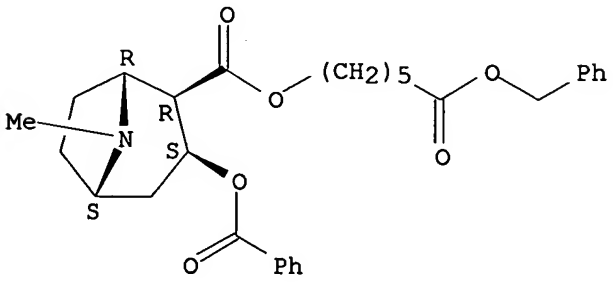
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 6-oxo-6-(phenylmethoxy)hexyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



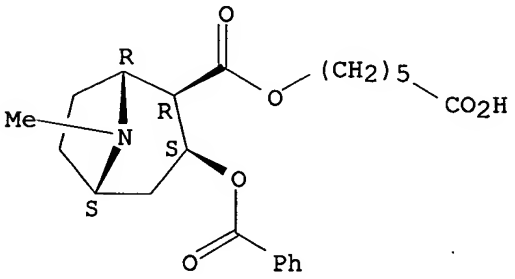
RN 173443-26-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 6-oxo-6-(phenylmethoxy)hexyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 173443-27-1 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 5-carboxypentyl ester, (1R,2R,3S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:966992 CAPLUS
DN 124:106527
TI Generation of polyclonal catalytic antibodies against cocaine using transition state analogs of cocaine conjugated to diphtheria toxoid
AU Basmadjian, Garo P.; Singh, Satendra; Sastrodjojo, Budiono; Smith, Blaine T.; Avor, Kwasi S.; Chang, Fengchun; Mills, Stanley L.; Seale, Thomas W.
CS Coll. Pharmacy, Univ. Oklahoma Health Sci. Cent., Oklahoma City, OK, 73117, USA
SO Chemical & Pharmaceutical Bulletin (1995), 43(11), 1902-11
CODEN: CPBTAL; ISSN: 0009-2363
PB Pharmaceutical Society of Japan
DT Journal
LA English
AB Six novel transition state analogs (TSAs) of cocaine and one non-cocaine, p-aminophenylphosphonyl ester of cyclohexanol, were prepared and characterized by 1H- and 13C-NMR and FAB-MS, (1R)-ecgonine Me ester or cyclohexanol were subjected to phenylphosphonylation in the presence of

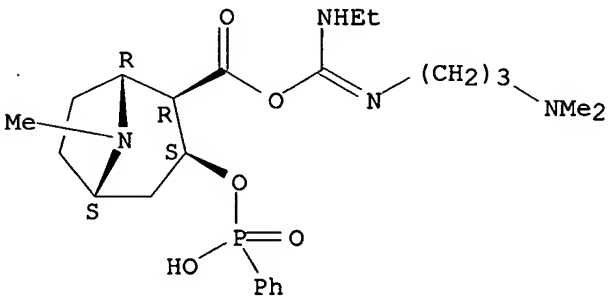
dicyclohexyl carbodiimide and 4-N,N-dimethyl aminopyridine. TSA-IV, however, was prepared from norcocaine which was protected with dibromoethane before acid hydrolysis, esterification and phenylphosphonylation were carried out. TSA-III, and TSA-I using various length spacer arms, were coupled with the immunogenic protein, diphtheria toxoid (DT). The TSAs coupled with DT were used to immunize mice and after appropriate boosts their sera were tested for the presence and titer of anti-TSA polyclonal antibodies using ELISA. The mice immunized with these TSAs produced high titers of polyclonal catalytic antibodies, except for 1 compound, with the ability to hydrolyze the substrate 125I-4'-iodococaine in an in vitro assay, even in the presence of noncatalytic anti-TSA antibodies.

IT **172954-58-4DP**, reaction products with diphtheria toxoid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(generation of polyclonal catalytic antibodies against cocaine using transition state analogs)

RN 172954-58-4 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(hydroxyphenylphosphinyl)oxy]-8-methyl-, anhydride with N-[3-(dimethylamino)propyl]-N'-ethylcarbamimidic acid, monohydrochloride, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



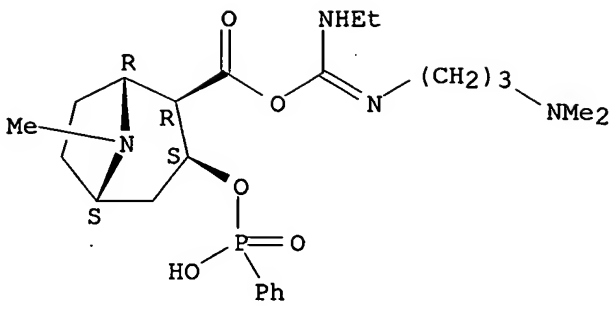
● HCl

IT **172954-58-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(generation of polyclonal catalytic antibodies against cocaine using transition state analogs)

RN 172954-58-4 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-[(hydroxyphenylphosphinyl)oxy]-8-methyl-, anhydride with N-[3-(dimethylamino)propyl]-N'-ethylcarbamimidic acid, monohydrochloride, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

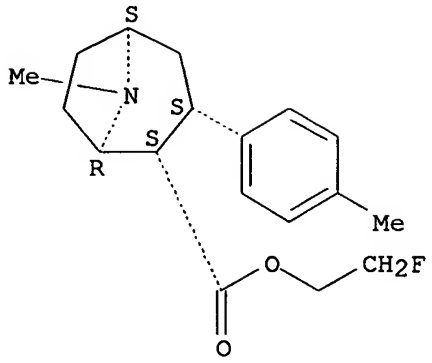
Absolute stereochemistry.
Double bond geometry unknown.



● HCl

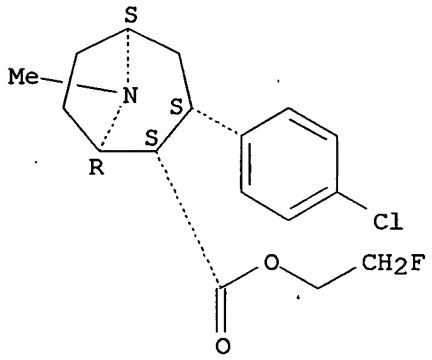
L5 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:701536 CAPLUS
DN 123:339691
TI Synthesis of two radiofluorinated cocaine analogs using distilled 2-[18F]fluoroethyl bromide
AU Wilson, Alan A.; Dasilva, Jean N.; Houle, Sylvain
CS Dep. Psychiatry, Univ. Toronto, Toronto, ON, M5T 1R8, Can.
SO Applied Radiation and Isotopes (1995), 46(8), 765-70
CODEN: ARISEF; ISSN: 0969-8043
PB Elsevier
DT Journal
LA English
AB Two fluorinated congeners of cocaine, 2'-fluoroethyl (1R-2-exo-3-exo)-8-methyl-3-(4-methylphenyl)-8-azabicyclo[3.2.1]octane-2-carboxylate (FETT) and its 4-chlorophenyl analog (FECT) were synthesized. Radiolabeling with 18F was achieved by O-[18F]fluoroalkylation of the corresponding carboxylic acid salts with distilled 2-[18F]fluoroethyl bromide in DMF. After HPLC purification, yields of radiochem. pure, formulated products were 22-30% (not corrected for decay) in a synthesis time of 60-70 min. The use of distilled 2-[18F]fluoroethyl bromide was indispensable for the reliable production of pure products.
IT **170163-96-9P 170163-97-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of cocaine analogs)
RN 170163-96-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, 2-fluoroethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



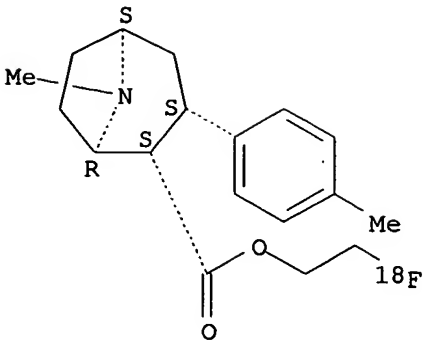
RN 170163-97-0 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, 2-fluoroethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



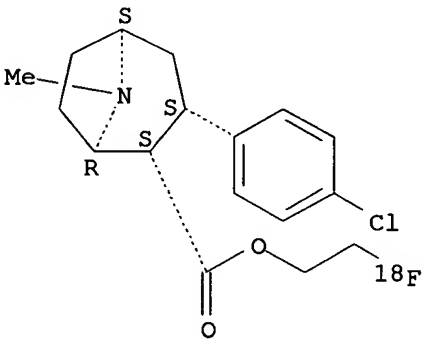
IT **170163-94-7P 170163-95-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of radiofluorinated cocaine analogs using distilled 2-[18F]fluoroethyl bromide)
RN 170163-94-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 8-methyl-3-(4-methylphenyl)-, 2-(fluoro-18F)ethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 170163-95-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(4-chlorophenyl)-8-methyl-, 2-(fluoro-18F)ethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



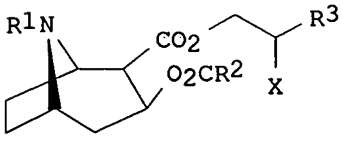
L5 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:656105 CAPLUS
DN 121:256105
TI Derivatives of benzoylecgonine, ecgonine and ecgonidine as medicines
IN Somers, Lowell M.; Wynn, James E.
PA Entropin, Inc., USA
SO PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9415935	A1	19940721	WO 1993-US12625	19931223
	W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5376667	A	19941227	US 1992-999307	19921231

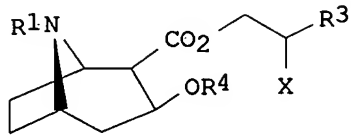
	CA 2151618	AA	19940721	CA 1993-2151618	19931223
	CA 2151618	C	20000801		
	AU 9460160	A1	19940815	AU 1994-60160	19931223
	AU 682677	B2	19971016		
	EP 677051	A1	19951018	EP 1994-906466	19931223
	EP 677051	B1	20011128		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	HU 72972	A2	19960628	HU 1995-2008	19931223
	JP 08507751	T2	19960820	JP 1993-516076	19931223
	JP 2938188	B2	19990823		
	PL 174826	B1	19980930	PL 1993-321837	19931223
	PL 175756	B1	19990226	PL 1993-309664	19931223
	AT 209646	E	20011215	AT 1994-906466	19931223
	PT 677051	T	20020531	PT 1994-906466	19931223
	ES 2169067	T3	20020701	ES 1994-906466	19931223
	IL 108193	A1	19981206	IL 1993-108193	19931227
	ZA 9309807	A	19940818	ZA 1993-9807	19931230
	CN 1095720	A	19941130	CN 1993-121730	19931230
	CN 1053187	B	20000607		
	US 5559123	A	19960924	US 1994-320050	19941007
	US 5663345	A	19970902	US 1995-463123	19950605
	NO 9502611	A	19950830	NO 1995-2611	19950629
	NO 313830	B1	20021209		
	HK 1012627	A1	20021004	HK 1998-113935	19981217
PRAI	US 1992-999307	A	19921231		
	WO 1993-US12625	W	19931223		
	US 1994-320050	A3	19941007		

OS MARPAT 121:256105

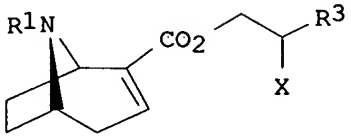
GI



I



II



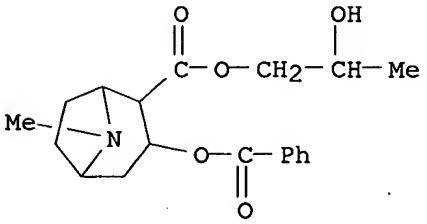
III

AB The title compds. [I; R1 = (un)branched alkyl, H, alkenyl, alkynyl; R2, R3 = (un)branched (un)substituted alkyl, alkenyl, alkynyl; X = OH, SH, NH2, halogen] [II; R4 = H, (un)substituted (un)branched alkyl, alkenyl, alkynyl] (III), useful in the treatment of pain, inflammation, autoimmune diseases, allergies, arthritis, gangrene, diabetes, etc., are prepared Thus, cocaine base was heated in an aqueous solution of propylene glycol, producing benzoylecgonine, ecgonine, ecgonidine, 2-hydroxypropylbenzoylecgonine, 2-hydroxypropylecgonine, and 2-hydroxyporpylecogonidine, and this mixture was successfully used in the treatment of patients suffering from a variety of the above-mentioned

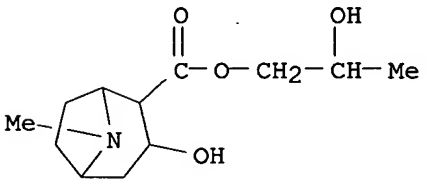
illnesses.

IT **157770-50-8P 157770-51-9P 157770-52-0P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as pharmaceutical)

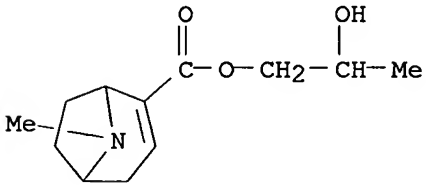
RN 157770-50-8 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2-hydroxypropyl ester (9CI) (CA INDEX NAME)



RN 157770-51-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, 2-hydroxypropyl ester (9CI) (CA INDEX NAME)



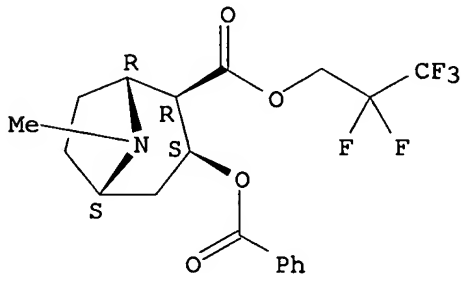
RN 157770-52-0 CAPLUS
CN 8-Azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid, 8-methyl-, 2-hydroxypropyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:451978 CAPLUS
DN 113:51978
TI Variations in abundance of the molecular ion of the derivatized cocaine metabolite benzoylecgonine
AU Bodor, Geza; Roggeman, Robert; Turk, John

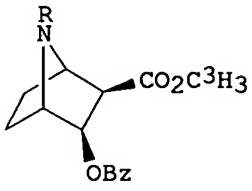
CS Sch. Med., Washington Univ., St. Louis, MO, 63110, USA
SO Clinical Chemistry (Washington, DC, United States) (1990), 36(5), 742-7
CODEN: CLCHAU; ISSN: 0009-9147
DT Journal
LA English
AB Benzolecgonine (BEG) is the principal urinary metabolite of cocaine. For forensic drug testing, the presence of BEG in urine, suggested by a pos. result for a screening immunoassay, must be confirmed by quant. gas chromatog./mass spectrometric (GC/MS) anal., i.e., stable isotope dilution with a deuterium-labeled internal standard GC/MS criteria for positivity also require appropriate relative abundances of qualifier ions, including the mol. ion, but there is little published information on the observed absolute values for qualifier ion ratios or on the variability of these values. This lack of information creates uncertainty for labs. initiating programs testing urine for drugs of abuse as to performance criteria for run acceptability and sample positivity. The authors have observed substantial variability (CV = 50%) in the abundance of the mol. ion of derivatized BEG relative to the base ion in reference materials. This variability can result in a high rate of repetition of runs and generate confusion in the defense of forensic drug-testing results. Normalization of the abundance of the mol. ion of derivatized BEG to that of the deuterium-labeled internal standard in the same sample greatly reduces the apparent variability in this measurement; it is also more reliable than the absolute value of the relative abundance of the mol. ion in determining run acceptability and pos. or neg. results for a sample.
IT **128429-28-7**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in human urine by GC/mass spectrometry in forensics)
RN 128429-28-7 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, 2,2,3,3,3-pentafluoropropyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1977:5653 CAPLUS
DN 86:5653
TI Radiosynthesis of (-)-cocaine and nor-(-)-cocaine using tritium-labeled methanol
AU Just, Wilhelm W.; Werner, Gottfried
CS Max Planck Inst. Hirnforsch., Arbeitsgruppe Neurochem., Frankfurt/Main, Fed. Rep. Ger.
SO Journal of Labelled Compounds and Radiopharmaceuticals (1976), 12(2),

281-5
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA English
GI



I

AB Hydrolysis of (-)-cocaine and (-)-norcocaine gave (-)-O-benzoylecgonine and (-)-O-benzoylnorecgonine, resp., which were converted to the corresponding acid chlorides and then treated with C3H3OH in MeCN to give 3H labeled cocaine and norcocaine (I; R = Me, H, resp.) with specific activity 90 and 38 mCi/mole, resp. I (R = H) was converted to its 1-N-dimethylaminonaphthalene-5-sulfonyl derivative

IT **61194-40-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61194-40-9 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-, trifluoromethyl ester, [1R-(exo,exo)]- (9CI) (CA INDEX NAME)